일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INTL-1**
발표분야: [대한화학회 창립 70주년, 한국화학연구원 창립 40주년 기념 국제심포지엄] Chemistry: Perspectives for the Future
발표종류: 특별강연, 발표일시: 수 13:30, 좌장: 김종승

Simple/Low-cost Bioanalysis for the Developing World and Point of Care

George M. Whitesides

Department of Chemistry and Chemical Biology, Harvard University, USA

This talk will describe exploratory research designed to develop systems based on first-world science to solve diagnostic problems in resource-limited environments, and to provide tools for public health. The work focuses on bioanalytical systems for diagnostics, and includes work on paper diagnostics, magnetic levitation, two-phase polymer systems, and electrochemistry. The program also has an unusual component, in asking what strategies in academic research will be most successful in converting results from university bench science into real solutions to problems in health in the hands of users.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INTL-2**
발표분야: [대한화학회 창립 70주년, 한국화학연구원 창립 40주년 기념 국제심포지엄] Chemistry: Perspectives for the Future
발표종류: 특별강연, 발표일시: 수 14:10, 좌장: 김종승

Single-Molecule, Single-Particle Chemistry of Nanocatalysts for Light Energy Conversion

Tetsuro Majima

The Institute of Scientific and Industrial Research (SANKEN), Osaka University, Mihogaoka 8-1, Ibaraki, Osaka 567-0047, Japan

To design an efficient light energy conversion system, it is important to reveal and understand the molecular interactions and the mechanism of chemical reactions at the heterogeneous interfaces. We have investigated the light energy conversion processes occurring on a variety of nanocatalysts using single-molecule, single-particle fluorescence imaging techniques and gain information related to spatial and temporal heterogeneities in reactions, which are always masked by ensemble averaging.

We synthesized novel fluorogenic probes to selectively observe the catalytic reactions. Such probes are designed to become fluorescent upon the reaction with target species under photoirradiation. The position of individual fluorescent products can be determined with several tens nanometers spatial resolution by two-dimensional Gaussian fitting. In addition, the quantitative analysis of fluorescence intensity trajectory or fluctuation can reveal the underlying properties of individual catalysts

We prepared nanometer- and micrometer-sized crystals of photoactive metal oxide semiconductors, such as titanium dioxide and bismuth vanadium oxide, and explore the photocatalytic reactions on individual catalysts by single-molecule fluorescence microscopy with newly developed redox-responsive fluorogenic probes. The effects of probe concentration, solvent, pH, and light intensity will be examined to optimize the experimental conditions. From the analysis of spatial distribution of reactive sites, the relationship between surface structures and chemical reactivity is elucidated. From the quantitative analysis of on/off duration times, we further determined the turnover frequency of individual catalysts, adsorption and dissociation rates, interfacial electron transfer rates, and temporal fluctuation of reaction efficiency.

The photochemical reaction dynamics of metal nanoparticles and various nanostructured materials are also studied at the ensemble and single-molecule and single-particle levels with the aid of quantum calculations to examine their possible use as nanocatalysts. We believe the proper understanding of structures and reactions at heterogeneous interfaces leads to the emerging applications of nanocatalysts for environmentally and economically sustainable uses.

References

1. T. Tachikawa, S. Yamashita, T. Majima, J. Am. Chem. Soc. 133 (2011) 7197.
2.T. Tachikawa, T. Yonezawa, T. Majima, ACS Nano 7 (2013) 263-275.
3. Z. Bian, T. Tachikawa, P. Zhang, M. Fujitsuka, T. Majima, Nat. Commun. 5 (2014) 4038/1.
4.Z. Bian, T. Tachikawa, P. Zhang, M. Fujitsuka, T. Majima, J. Am. Chem. Soc. 136 (2014) 458.
5.P. Zhang, T. Tachikawa, M. Fujitsuka, T. Majima, Chem. Commun. 51 (2015) 7187.
6. P. Zhang, T. Tachikawa, M. Fujitsuka, T. Majima, J. Phys. Chem. Lett. 7 (2016) 1173-1179.
7. Z. Zheng, T. Tachikawa, T. Majima, J. Am. Chem. Soc. 136 (2014) 6870.
8. Z. Zheng, T. Tachikawa, T. Majima, J. Am. Chem. Soc. 137 (2015) 948.
9. Z. Zheng, T. Tachikawa, T. Majima, Chem. Commun. 51 (2015) 14373.
10. Z. Zheng, T. Majima, Angew. Chem. Int. Ed. 55 (2016) 2879-2883.
11. Z. Lou, M. Fujitsuka, T. Majima, ACS Nano DOI: 10.1021/acsnano.6b02494.

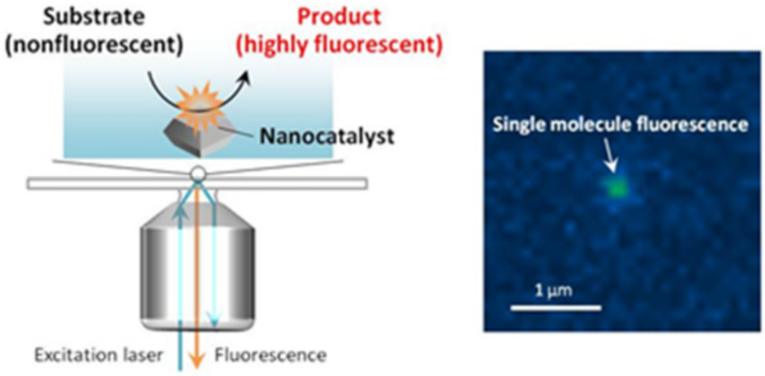


Figure 1 Single-molecule fluorescence imaging of photocatalytic reactions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INTL-3**
발표분야: [대한화학회 창립 70주년, 한국화학연구원 창립 40주년 기념 국제심포지엄] Chemistry: Perspectives for the Future
발표종류: 특별강연, 발표일시: 수 14:50, 좌장: 김종승

Nanoscale Gems, Needles and Grooves: New Material Platforms for Physical and Life Science Research

Hongkun Park

Department of Chemistry and Chemical Biology and Department of Physics, Harvard University Broad Institute of Harvard and MIT, USA

My laboratory leverages our chemistry expertise to develop new nanoscale materials and tools and apply them to a variety of problems ranging from quantum information processing, plasmonics, nano-bio interfacing, all the way to single-cell sequencing. In this presentation, I will describe recent examples of such efforts based on three nanoscale structures – diamond nanocrystals, silicon needles and silver grooves – and how we use them to address various problems in physical and life sciences. First, I will discuss our efforts to combine two-dimensional plasmonic crystals and metasurfaces, silicon-vacancy centers in nanostructured diamond, and two-dimensional transition metal dichalcogenides to realize integrated all-optical devices and logic circuits that work all the way down to the single-photon level. Next, I will present diamond nanocrystals containing the nitrogen-vacancy color centers: these nanocrystals can not only serve as solid-state atom-like qubits that can be coupled to the photonic/plasmonic structures, but also function as ultrasensitive electromagnetic and temperature sensors that can be coupled to living systems. Finally, I will discuss a CMOS-nanoneedle electrode array that enables highly multiplexed interrogation and manipulation of mammalian cells in a minimally invasive fashion. These examples illustrate how the developments of new nanoscale structures and tools enable new lines of scientific inquiries.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INTL-4**

발표분야: [대한화학회 창립 70주년, 한국화학연구원 창립 40주년 기념 국제심포지엄] Chemistry: Perspectives for the Future

발표종류: 특별강연, 발표일시: 수 16:10, 좌장: 이창진

Bioinspired Functional Surfaces – A Challenge for Interdisciplinary Materials Research

Eduard Arzt

Scientific Director and Chairman (CEO), INM - Leibniz Institute for New Materials; and Professor for New Materials, Saarland University, Campus D2 2, 66123 Saarbruecken, Germany

New surfaces and coatings can drastically improve the properties and applicability of materials. At INM, we develop and investigate new dynamic surfaces for diverse functionalities: low friction, adhesion, corrosion protection, anti-reflection, electric storage and combinations of these. Such surfaces either exhibit new chemistries or new fibrillar topographies, sometimes on different hierarchical levels. I will give an overview of some of our recent developments in these areas. Then I will highlight our bio-inspired exploitation of the “gecko effect”: after research over more than a decade, also on living animals, we are now in a position to artificially produce and optimize such surface protrusions to create also switchable functionalities. Recently, we investigated such features numerically by considering the micromechanics of detachment of single elastic fibrils from an elastic half-space; the simulations now guide the fabrication of such surfaces with promising applications in robotics, sports devices and biomedicine.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INTL-5**

발표분야: [대한화학회 창립 70주년, 한국화학연구원 창립 40주년 기념 국제심포지엄] Chemistry: Perspectives for the Future

발표종류: 특별강연, 발표일시: 수 16:50, 좌장: 이창진

Necessity for Sophisticated Chemical Synthesis: Doing What we Must, Not What we Can

Amir H. Hoveyda

Boston College, Department of Chemistry, Merkert Chemistry Center, Chestnut Hill, Massacussetts, 02467, USA

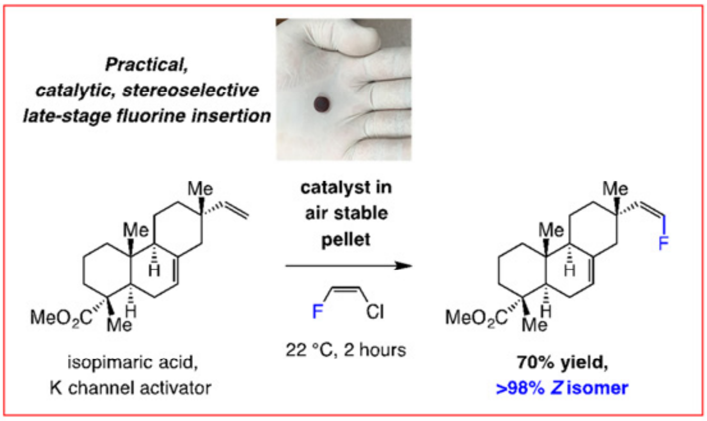
Chemical synthesis, while enabling us to access molecules as efficiently as possible, can expand our understanding of the fundamental principles of reactivity and selectivity. It gives us the opportunity of examining molecules that we imagine to be special and brings us molecules that are on our “wish list” – it gives us the opportunity to wonder “what if?”. Significant advances have indeed been achieved, but to consider the whole of organic synthesis a consummated field would be akin to suggesting to the great Henry Ford that his model T was the be-all and end-all in automobile making. It is likely true that an expert chemist, given sufficient amount of time and funds, could prepare almost any molecule in a specially-equipped laboratory, but often only as morsels, after suffering countless wrong turns and myriad dead-ends. For synthetic chemistry to provide the impact that it can many crucial advances must be realized. This lecture will focus on some of these issues.

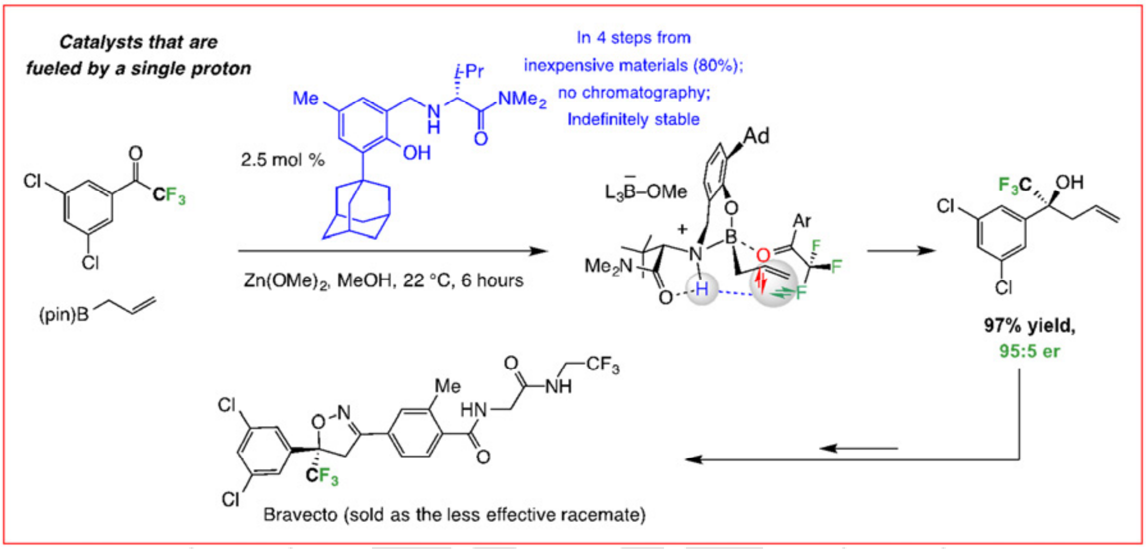
References

1.Koh, M. J.; Nguyen, T. T.; Zhang, H.; Schrock, R. R.; Hoveyda, A. H. Nature 2016, 531, 459.

2.Nguyen, T. T.; Koh, M. J.; Shen, X.; Romiti, F.; Schrock, R. R.; Hoveyda, A. H. Science 2016, 352, 569.

3.a) Silverio, D. L.; Torker, S.; Palyugina, T.; Vieira, E. M.; Snapper, M. L.; Haeffner, F.; Hoveyda, A. H. Nature 2013, 494, 216. b) Lee, K.; Silverio, D. L.; Torker, S.; Haeffner, F.; Robbins, D. W.; Hoveyda, A. H. Nature Chem. 2016, 8, 768.


Practical, catalytic, stereoselective late-stage fluorine insertion
Me
Me
H
H
MeO2C
Me
isopimaric acid, K channel activator
catalyst in air stable pellet
F
Cl
22 °C, 2 hours
Me
Me
H
F
H
MeO2C
Me
70% yield,
>98% Z isomer


Catalysts that are fueled by a single proton
Cl
O
CF3
Cl
(pin)B
Me
i-Pr
N
H
NMe2
O
OH
2.5 mol %
In 4 steps from inexpensive materials (80%); no chromatography; Indefinitely stable
Zn(OMe)2, MeOH, 22 °C, 6 hours
Ad
L3B–OMe
O
+
B
Ar
O
Me2N
N
F
F
O
H
F
F3C
OH
Cl
Cl
97% yield,
95:5 er
Cl
O
N
Me
O
CF3
HN
NH
CF3
Cl
CF3
O
Bravecto (sold as the less effective racemate)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INTL-6**
발표분야: [대한화학회 창립 70주년, 한국화학연구원 창립 40주년 기념 국제심포지엄] Chemistry: Perspectives for the Future
발표종류: 특별강연, 발표일시: 수 17:30, 좌장: 이창진

Stitching and Weaving of Molecules into New Materials

Omar M. Yaghi

Department of Chemistry, University of California-Berkeley, Berkeley, CA, United States

The most important materials humanity has known are made entirely from either organic or inorganic components. Until recently the development of crystalline materials in which organic and inorganic are combined remained largely unexplored. This presentation will discuss the key developments in the discovery of new materials based on stitching and weaving organic and inorganic molecules into framework structures – the arts and sciences of Reticular Chemistry, and highlight how this class of new crystalline materials has come to represent the largest class of materials ever made and currently being pursued by academia and industry.

Specifically, the chemistry of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) is based on linking molecular building units into extended covalent porous crystals using covalent bonds such as M-O, C-O, B-O, and C-N. These new classes of materials have many applications related to energy storage, carbon dioxide capture and conversion, super capacitors, to mention few. This presentation will also focus on the making of MOFs and COFs by covalent chemistry as well as the post synthesis covalent modification of these to produce precisely designed interiors capable of selective carbon dioxide capture, water capture from air to produce fresh water, and catalysis. The idea of incorporating sequences of chemical information within MOFs and COFs to code for specific properties will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **AWARD-1**
발표분야: 기념강연
발표종류: 기념강연, 발표일시: 목 16:00, 좌장: 이덕형

Nucleophilic fluorination: Is it possible at room temperature?

지대윤

서강대학교 화학과

Incorporation of fluorine-18 into big biomolecules such as proteins, oligopeptides, oligonucleotide, dendrimers, or antibodies is a burgeoning field with more widely used as in vivo imaging agents. We have developed new fluorination method using 1,2,3-triazolium salts. Triazolium salts play a crucial role in shortening reaction time, increasing radiochemical yield, lowering reaction temperature, and water solubility. Now we had a successful results of the fluorination by nucleophilic substitution reactions at room temperature within 1 min. The water-soluble property of fluorinated triazolium salt would allow bioconjugation reaction efficiently in aqueous media to proceed faster under mild condition.

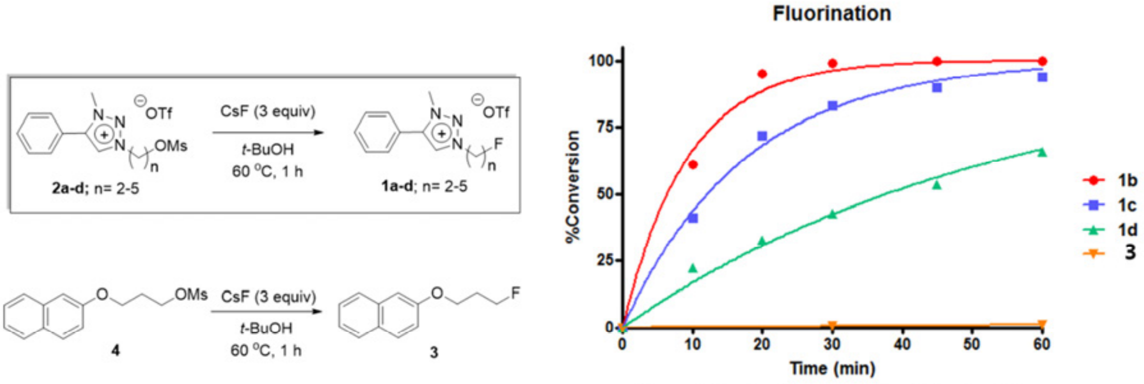


Figure. Fluorination reactivity of **2a-d** and **4**.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY1-1**

발표분야: Nucleic Acids in Materials Science – Programmable Biopolymers

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김원종

Layer-by-Layer Assembly for Graphene-Based Multilayer Nanocomposites: Multilayered opportunity

김병수

UNIST 화학과

Carbon nanomaterials including fullerenes, carbon nanotubes, and graphenes represent the most important class of materials today; their unique physical and chemical attributes advance their roles across most advanced scientific and technology platforms. Among them, chemically exfoliated version of graphene, graphene oxide nanosheets are receiving interests for their various surface functional groups while preserving some intrinsic properties of graphene. In this presentation, I will describe the efforts of past 7 years in developing graphene-based hybrid nanomaterials based on layer-by-layer (LbL) self-assembly techniques. LbL assembly has been widely used as a versatile method for fabricating multilayer thin films of various materials with a controlled architecture and composition at a nanometer scale precision. Specifically in this talk, I will illustrate the hierarchically self-assembled graphene superstructures for potential material applications such as transparent conducting thin films, transistors, electrocatalysts, and biosensors. In addition, the tunable nature of graphene oxide in terms of surface charge and dimension for the controlled assembly will be discussed with a future prospective in the area.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY1-2**
발표분야: Nucleic Acids in Materials Science – Programmable Biopolymers
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 정유진

Dynamic Nanostructures Fabricated from DNA Block Copolymers

박소정* **Qingjie Luo[1]**

이화여자대학교 화학나노과학과 [1]University of Pennsylvania

Here, we present active DNA nanostructures fabricated through the self-assembly of DNA block copolymers. A DNA diblock copolymer of polymethylacrylate-block-DNA (PMA-b-DNA) were synthesized and co-assembled with a prototypical amphiphilic polymer of poly(butadiene)-block-poly(ethylene oxide) (PBD-b-PEO).1 The binary self-assembly of PMA-b-DNA and PBD-b-PEO resulted in giant polymersomes with DNA uniformly distributed in the hydrophilic PEO shell. When giant polymersomes were connected through specific DNA interactions, DNA block-copolymers migrated to the junction area, forming DNA islands within polymersomes. These results indicate that DNA hybridization can induce effective lateral polymer segregation in mixed polymer assemblies. The polymer segregation and local DNA enrichment has important implications in DNA melting properties, as mixed block copolymer assemblies with low DNA block copolymer contents can still exhibit useful DNA melting properties that are characteristic of DNA nanostructures with high DNA density. The presentation will also discuss ways to prepare shape-changing dynamic nanostructures through DNA-based self-assembly.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY1-3**

발표분야: Nucleic Acids in Materials Science – Programmable Biopolymers

발표종류: 심포지엄, 발표일시: 목 14:25, 좌장: 정유진

Conjugated polymer and aptamer based fluorescence chemo- and bioassays

정지은 우한영*

고려대학교 화학과

Conjugated polyelectrolytes (CPEs) are described by a π-conjugated backbone with ionic pendant groups, which make them water-soluble and/or bio-compatible. Here, we report a new potassium ion detection assay using a molecular beacon aptamer (MBA) and CPEs. The K^+-specific aptamer sequence in MBA was used as a molecular recognition element. The hairpin-type MBA labeled with a fluorophore and quencher at both termini undergoes a conformational change (by complexation with CPEs) to either an open-chain form or a G-quadruplex in the absence or presence of K^+ ions. Conformational changes of MBA as well as signal quenching or amplification via fluorescence resonance energy transfer (FRET) from CPEs provide clear signal trun-off and –on in the presence or absence of K^+. Combination of high binding specificity of MBA and synthetic CPEs with tunable optical amplification property provided the ultimate detection sensitivity and selectivity. The successful detection of 5'-adenosine triphosphate (ATP) and tuning of detection range with a series of MBAs containing an ATP-specific aptamer sequence was also demonstrated using the same sensor scheme. In addition, a series of inhibitors were incorporated to modulate the detection range of MBA-based assay.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY1-4**
발표분야: Nucleic Acids in Materials Science − Programmable Biopolymers
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 정유진

Tumor targeting delivery system for polymerized siRNA

김광명

한국과학기술연구원(KIST) 의공학연구소

Gene expression control by the small interfering RNA (siRNA) is a most promising tool for gene therapy by sequence specific cleavage of mRNA. But siRNA's instability and poor cell penetrating properties are being obstacles for its application. So, it requires effective siRNA delivery system for diverse use. Here we present the new carrier which composed of biocompatible/biodegradable glycol chitosan based nanoparticles (NP) for complex formation with siRNA. Using the Red Fluorescence Protein (RFP) over-expressed mouse melanoma B16F10 cells and athymic nude mouse, delivery effects of NP-siRNA were examined such as fluorescence imaging methods for cellular uptake, gene silencing efficacy and biodistribution etc. Although the development of various gene delivery systems has increased the siRNA delivery efficiency, still many problems remain to be resolved before the clinical application of siRNA. So, we suggest reducible polymerized siRNA a possible solution for low delivery efficiency of siRNA. By increasing the size of siRNA, poly-siRNA formed more condensed and nano-sized complexes due to strong electrostatic interaction, we obtained enhanced cellular uptake of siRNA and powerful gene silencing effect. Our results demonstrate that strong polyanionic, reducible poly-siRNA can serve as a powerful therapeutic agent for treating human diseases.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY1-5**

발표분야: Nucleic Acids in Materials Science – Programmable Biopolymers

발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 정유진

Aligned DNA molecules and its applications

윤동기

KAIST 나노과학기술대학원

Organization of biopolymer is significant for not only an evolution of a biological system but also construction of material for well-defined nanostructures. Recently, several researchers have investigated a formation of liquid crystalline pattern of semi-flexible biopolymers such as a DNA and Sunset yellow (SSY).[1,2] However, the pattern of biopolymers was formed on restricted area that makes this intriguing patterns hard to utilize in useful applications.Here, we produced liquid crystalline patterns of DNA in drying process induced from the shear-aligning process. The aligned patterns were analyzed by polarized optical microscopy (POM) and atomic force microscopy (AFM). The pattern in large area can provide applications to bio-template for nanoparticles or other biomaterials and electrical nano-device. References[1] L. Vonna et al., Langmuir, 21, 9635-9643 (2005).[2] I. I. Smalyukh et al., PRL 96, 177801 (2006).[3] Y. J. Cha et al., ACS Appl. Mater. Inter., 7, 13627 (2015).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY2-1**
발표분야: Architecture Controlled Polymers: Dendrimer, Hyperbranched, Star, Cycle and beyond
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 김병수

Synthesis of well-defined amphiphilic topological block copolymers via super base-catalyzed ring-opening polymerization of epoxide

Toshifumi SATOH

Faculty of Engineering, Hokkaido University, Japan

The synthesis of well-defined amphiphilic topological block copolyethers (star, cyclic, figure-eight-shaped, tadpole-shaped, and trefoil-shaped BCPs) together with the linear BCP counterpart were achieved by the *t*-Bu-P_4-catalyzed block copolymerization of decyle glycidyl ether (DGE) and triethylene glycol glycidyl methyl ether (TEGGE). The four-armed star-block copolyether was synthesized by the sequential *t*-BuP_4-catalyzed block copolymerization of DGE and TEGGE using the tetra-alcohol initiator according to the core-first method. The synthesis of the miktoarm star copolyethers was achieved by the combination of the *t*-BuP_4-catalyzed ring-opening polymerizwtion and intermolecular click reaction of the precursor polyethers. The synthesis of cyclic, figure-eight-shaped, and trefoil-shaped BCPs were carried out through three reaction steps; (i) *t*-Bu-P_4-catalyzed block copolymerization of DGE and TEGGE using the alcohol which have azido groups as an initiator, (ii) ω-end functionalization using propargyl bromide, and (iii) intramolecular cyclization using click reaction. The tadpole-shaped BCP was synthesized by five steps; (i) *t*-Bu-P_4-catalyzed polymerization of DGE using 3-phenyl-1-propanol as an initiator (PDGE), (ii) synthesis of PDGE with an azido and a hydroxyl group at ω-chain end (PDGE-(N_3)-OH), (iii) *t*-Bu-P_4-catalyzed post-polymerization of TEGGE using PDGE-(N_3)-OH as a macroinitiator, (iv) ω-end propargylation, and (v) intramolecular click cyclization. The products were identified to be targeted star, cyclic, figure-eight-shaped, tadpole-shaped, and trefoil-shaped BCPs by SEC, IR and ^{1}H NMR measurements. In addition, the number-average molecular weights (M_ns,$_{NMR}$) of BCPs were agreed with the calculated values based on initial monomers to initiator ratio, and the dispersitys of BCPs were narrow (1.04-1.08). In order to investigate the aggregation behavior of topological BCPs, the hydrodynamic diameter, the critical aggregation concentration, and the cloud point were determined by dynamic light scattering, fluorescence technique using pyrene, and variable-temperature UV-Vis absorption measuremant, respectively.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY2-2**
발표분야: Architecture Controlled Polymers: Dendrimer, Hyperbranched, Star, Cycle and beyond
발표종류: 심포지엄, 발표일시: 금 09:50, 좌장: 윤진환

Controlled Synthesis of Hyperbranched Polyglycerols and Their Potential Uses

김일

부산대학교 고분자공학과

Recently ring-opening multibranching polymerization (ROMBP) has been demonstrated as a versatile method for the synthesis of a variety of hyperbranched homopolymers as well as complex macromolecular architectures. Intense efforts have been undertaken to thoroughly characterize these molecules and optimize the synthetic pathway. Modulations of the initiator core and/or the multiple periphery end groups have revealed remarkable potential for applications such as liquid-crystalline materials, hydrogels, polyelectrolytes and hybrid materials for biomineralization. However, most of the previous reports are based on hyperbranched polyglycidols synthesized by the ROMBP of glycidol (dormant AB_2 monomer) using 1,1,1-tris(hydroxymethyl)propane (TMP), bearing three OH-groups, as a typical multifunctional initiator core in the presence of base catalyst.

As a means of expanding a versatility of hyperbranched polymers we designed a new hyperbranched polythioether (HPTE), bearing ether, thioether and hydroxyl groups throughout the matrix (Scheme 1). The resulting HPTEs were employed to template the preparation of TiO_2 by the sol-gel process in methanol without any additional surfactants. A series of biocompatible and degradable hyperbranched polyether esters, poly(2-hydroxyethyl 2-methyloxirane-2-carboxylate) (pHEMOC) with controlled molecular weight and polydispersity, have also been synthesized via ROMBP. The pHEMOCs comprised of ether and ester backbones and multiple hydroxyl groups on the core and periphery results in materials that exhibit good degradability and low cytotoxicity, enabling them to be an ideal candidate material for biomedical applications.

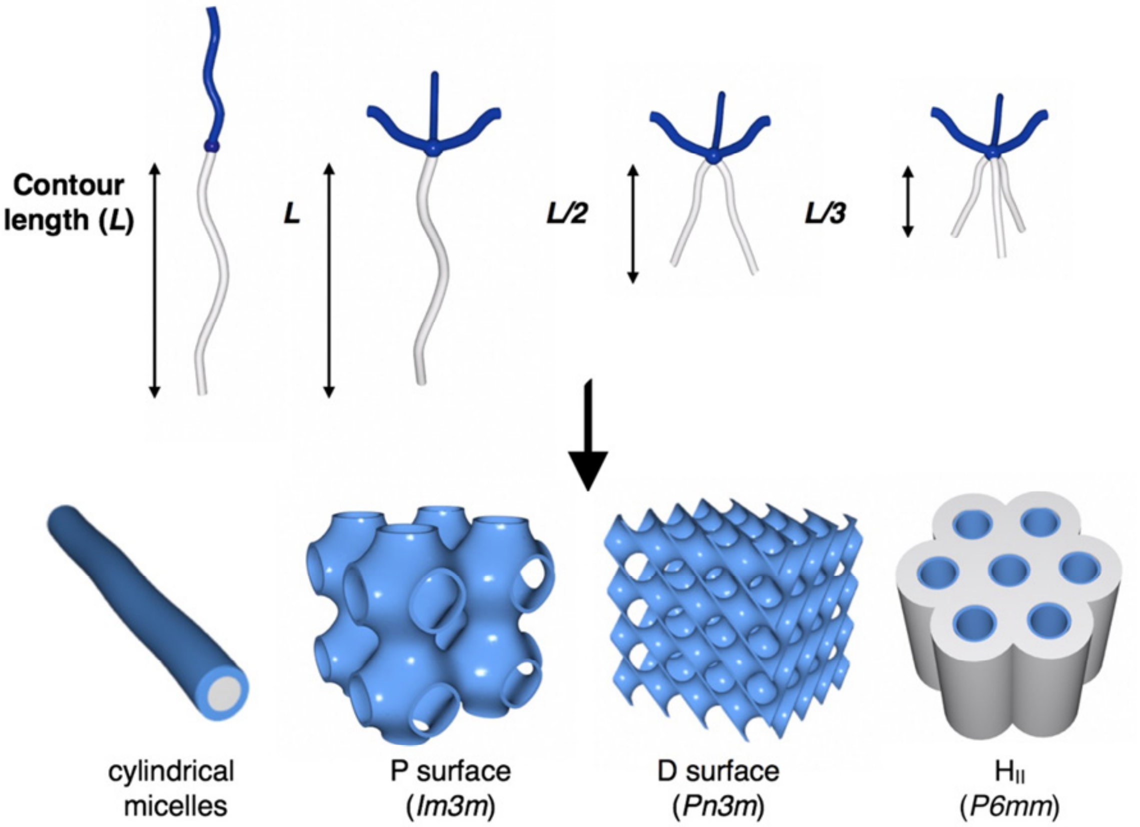
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY2-3**
발표분야: Architecture Controlled Polymers: Dendrimer, Hyperbranched, Star, Cycle and beyond
발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 윤진환

Branched Block Copolymers and Their Solution Self-Assembly

김경택

서울대학교 화학부

Inverse bicontinuous cubic (IBC) structures consisting of triply periodic minimal surfaces of block copolymers (BCPs) are emerging as materials of interest owing to their structural characteristics, which resemble those of their biological counterparts constructed from lipids. Solution self-assembly of amphiphilic BCPs with non-linear architectures have recently been shown to form colloidal particles (polymer cubosomes) and macroscopic monoliths having mesoporous networks of water channels embedded in the periodic minimal surfaces of the BCP bilayers. Here we report that BCP architectures play a crucial role in controlling the packing parameter (P) of BCPs; a value greater than unity is a prerequisite for preferential self-assembly into IBC mesophases in solution. We show that the branched architecture of the polymer blocks constituting the BCP critically influences the structural parameters, such as the molecular area and, in particular, the critical length of the hydrophobic domain. Adjusting these structural parameters not only increases the P value of the BCP without depending on the asymmetry of the volume ratio of two polymer blocks (block ratio), but also dictates the lattice and periodicity of the resulting minimal surfaces of the BCPs. Our results could provide a rationale to design and synthesize amphiphilic block copolymers to directly self-assemble into periodic porous structures in solution, which could be promising materials having highly ordered mesopore-networks.


Contour length (L)
L
$L/2$
$L/3$
cylindrical micelles
P surface ($Im3m$)
D surface ($Pn3m$)
H_{II} ($P6mm$)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY3-1**

발표분야: Flexible Thermoelectric Materials for Wearable Devices

발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 장광석

Flexible Thermoelectric Generator Using Organic Materials by Printing Process

조성윤

한국화학연구원 화학소재연구본부

Thermoelectric energy conversion is an attractive and environmentally friendly way to recover energy from industrial waste heat or natural heat because of its potential for improving the energy efficiency. As thermoelectric materials, organic materials have unique advantages, such as cost effectiveness, low intrinsic thermal conductivity, high flexibility, and amenability to large area applications. Therefore, organic conducting polymers, which possess good electrical conductivity, have been actively researched. Herein, we present a convenient method for enhancing the thermoelectric properties of inorganic-based nanostructures coated with poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) (PEDOT:PSS hybrid) by simple chemical treatment. Significant enhancement of the electrical conductivity of PEDOT:PSS hybrids was achieved by simple chemical treatment with H_2SO_4.The power factor of the developed materials could be effectively tuned over a very wide range depending on the concentration of the H_2SO_4 solution used in the chemical treatment. The power factors of the developed thermoelectric materials were optimized to 284 $\mu W\ m^{-1}\ K^{-2}$. Using the BiTe-PEDOT:PSS hybrids, a flexible thermoelectric generator that could be embedded in textiles was fabricated by a printing process. This thermoelectric array generates a thermoelectric voltage of 2 mV using human body heat

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY3-2**
발표분야: Flexible Thermoelectric Materials for Wearable Devices
발표종류: 심포지엄, 발표일시: 금 13:50, 좌장: 장광석

Nano- and molecular-solder introduced thermoelectric materials and device fabrication

손재성

UNIST 신소재공학부

Highly efficient thermoelectric materials have attracted tremendous attention due to various technological applications such as power generation from waste heat and environmentally friendly refrigeration. Recently, nanostructuring has become the core of thermoelectric (TE) material research because it creates numerous internal interfaces that provide an effective way to tune the thermal and/or electrical properties. Herein, we propose a new strategy for interface engineering of nanostructured TE materials by introducing chemically synthesized nanostructures or molecular compounds as solders. These solders easily fill up the voids and interfaces between TE particles and form crystalline phases to interconnect TE particles upon heat treatment with no external pressure, which led to huge densification and substantial growth of TE grains. The chemical design of solders allowed for the selective enhancement or reduction of the majority carrier concentration near the grain boundaries, and thus resulted in doped or de-doped inter-faces in granular BiSbTe material.Furthermore, the energy filtering effect could be realized by the formation of potential well at interfaces of BiSbTe grains. Finally, the low temperature sintering properties enabled us to design shapes and dimensions of TE materials and devices with high performance via a facile and cost-effective TE painting process.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY3-3**

발표분야: Flexible Thermoelectric Materials for Wearable Devices

발표종류: 심포지엄, 발표일시: 금 14:10, 좌장: 장광석

Rational design of Nanocarbon/Te nanowire composites for flexible thermoelectric materials

김희숙

KIST 광전하이브리드연구센터

As commercial interest in flexible power-conversion devices increases, the demand is growing for high-performance alternatives to brittle inorganic thermoelectric materials. As an alternative, we propose a flexible single-walled carbon nanotube (SWCNT)-doped tellurium nanowire (TeNW) hybrid film and rationally engineer the work function of the SWCNTs to effectively filter charge carriers in an energy-dependent manner at the interfaces between the carbon and the inorganic semiconductor. The acid treatment used to control the SWCNT work function allows the interfacial barrier between the SWCNT and the TeNW to be raised and lowered. While the hybrid film with a large barrier of 0.82 eV has a low power factor due to poor carrier transfer, the power factor (3.40 μW·m−1·K−2) in the film with a lower barrier of 0.23 eV is several times higher than that of either pure TeNW or hybrid film with 0.82 eV due to effective energy filtering effect. The transport characteristics of the hybrid film are explored to quantitatively elucidate the carrier filtering at the SWCNT-TeNW interfaces. As another alternative, we also demonstrate a rationally designed graphene/polymer/inorganic nanocrystal free-standing paper with high-TE performance, high-flexibility, and mechanical/chemical durability. The ternary hybrid system of graphene/polymer/inorganic nanocrystal introduces two heterojunctions to induce double-carrier filtering, thus increasing the electrical conductivity without a major decrease in the thermopower. The ternary hybrid shows 1~2 orders of magnitude higher power factor (143 μW·m-1·K-1) than either single or binary component and the maximum ZT of 0.2. We believe that the strategy proposed here to improve the performance of flexible thermoelectric materials by introducing more heterojunctions and optimizing carrier transfer at those junctions shows a great potential for the preparation of flexible/or wearable power conversion devices.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY3-4**
발표분야: Flexible Thermoelectric Materials for Wearable Devices
발표종류: 심포지엄, 발표일시: 금 14:40, 좌장: 조성윤

Fabrication of large and flexible organic thermoelectric module using stream-jet coating

이동준 김재윤[1] 곽정훈[1] 정병준*

서울시립대학교 신소재공학과 [1]서울시립대학교 전자전기컴퓨터공학부

Recently, organic thermoelectric (TE) devices based on conducting polymers and small molecules are attractive for wearable devices as a portable energy harvester. A famous conducting polymer in organic TE is the commercialized poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) specially PH1000 model of Clevios. Many researchers have reported the organic TE properties of PEDOT:PSS thin films through several treatments to improve Seebeck coefficient or electrical conductivity such as the chemical doping/dedoping, physical doping/dedoping, solvent annealing and acid treatments. PEDOT:PSS thin films have been usually fabricated on glass by spin-coating. The spin-coating method is useful for each PEDOT:PSS thin films to evaluate organic TE properties. To form PEDOT:PSS thin film on large plastic films such as PET and PEN, other coating processes will be investigated. In this presentation, we report the sorbitol-mixed PEDOT:PSS thermoelectric device and module using stream-jet coating. The unipolar serial connected module showed the Seebeck coefficient close to sum of those of individual devices.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY3-5**
발표분야: Flexible Thermoelectric Materials for Wearable Devices
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 조성윤

공액고분자-CNT 유기복합 열전소재 및 열전소자

장광석

한경대학교 화학공학과

열전소재는 지벡효과에 의해 폐열을 전기에너지로 변환시킬 수 있는 소재이기 때문에 그린 에너지 소재로 큰 관심을 받고 있다. 여러가지 열전소재 중에서도 최근에는 공액고분자를 바탕으로 한 유기 열전소재에 대한 연구가 큰 각광을 받고 있다. 유기 열전소재는 무기 열전소재에 비해 아직까지 성능이 매우 떨어지지만, 값싸고, 인쇄공정 적용이 가능하며, 유연소자로의 응용이 가능하다는 장점을 가지고 있다. 공액고분자의 경우 보통은 전기전도도가 낮기 때문에 열전특성이 낮은 경우가 많다. 공액고분자의 전기전도도 및 열전특성을 향상시키기 위해서 공액고분자를 CNT 와 복합화 시키는 연구가 진행되고 있다. 본 발표에서는 유연 열전소자로의 응용을 위한 공액고분자-CNT 잉크제조와 분산 기술에 대해 소개하고, 인쇄공정을 적용하여 유연, 유기복합 열전소자를 구현하는 연구내용을 소개하고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR1-1**

발표분야: Recent Trends in Inorganic Chemistry I: Symposium for Senior Professors

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이준승

Metallosupramolecualr Architectures based on 3,6-Disubstituted *s*-Tetrazine Ligands

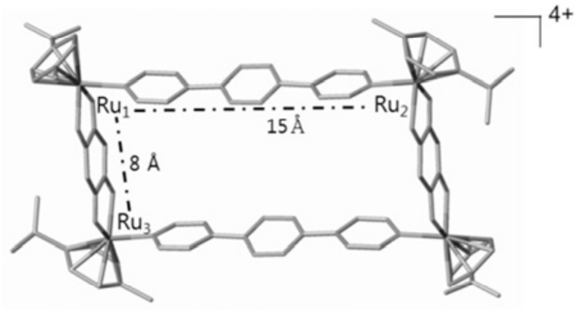
최문근

연세대학교 화학과

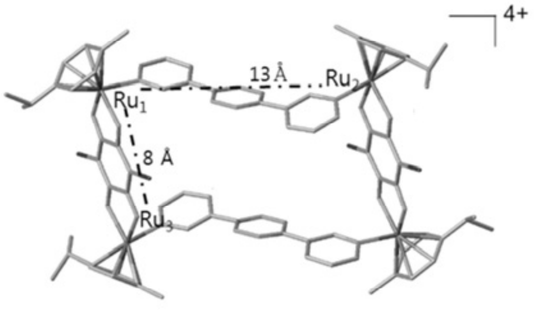
s-Tetrazines, six-membered aromatic heterocycles with four nitrogen, have extremely deficient π-electron system and are enable to sustain efficient attraction for polarized atoms or anions. In the view of coordination chemistry of *s*-tetrazines, their poor π-electron densities and multi coordination sites lead the structural diversity of coordination complexes depending on counter anions and electron rich guest molecules. In this study, a series of coordination polymers which consist of *s*-tetrazine ligands and silver(I) ions were synthesized and their structural diversity depending on counter anions were analyzed by single crystal X-ray diffractions. Furthermore two novel tetraruthenocycles containing structural isomers of bipyridyl-*s*-tetrazines (*p*-PTTz and *m*-PTTz) were synthesized and characterized by ^{1}H NMR and elemental analysis. The molecular structures of these ruthenocycles are determined by single crystal X-ray diffraction study. The structures of (*p*-PTTz-Ru and (*m*-PTTz-Ru exhibit rectangular shaped macrocycles with nano pores of 13 X 8 Å and 15 X 8 Å respectively, and their structural features were determined by the geometrical differences between *p*-PTTz and *m*-PTTz. These cavities are large enough to encapsulate polyaromatic molecules like anthracene, pyrene and phenanthrene. Especially extremely poor π-electron density of *s*-tetrazine rings affected efficient binding affinity of ruthenocycles with aromatic guest molecules through donor acceptor interactions. The binding constants between ruthenocycles and polyaromatic guests were measured by ^{1}H NMR in d_6-acetone.

The structural diversity of *s*-tetrazine Ag(I) coordination polymers depending on the nature of anion and the trend of binding constants between ruthenocycles and π -aromatic guests will be presented.

Figure 1. 3D structures of p-PTTz-Ru and m-PTTz-Ru



(*p*-PTTz-Ru)



(*m*-PTTz-Ru)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR1-2**
발표분야: Recent Trends in Inorganic Chemistry I: Symposium for Senior Professors
발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 이준승

Group 10 pseudo-halogen compounds: synthesis, reactivity, and catalytic application

김용주

강릉원주대학교 화학과

The azido (N3-) group coordinated to transition metals has been intensively studied for many years as one of the important pseudo-halogen ligands including CN, SCN, NCS, and NCO. The azido ligand coordinated to transition metals undergo thermal or photo induced reactions and 1,3-dipolar cycloaddition with organic unsaturated compounds, whereas halogeno compounds exhibit poorer chemical properties. Although extensive studies of transition azido complexes have been established, exploring group 10 metal azides with various functional ligands is still very interesting subject. Introducing the azido (N3) group including other pseudo-halogen ligands into the transition metal complexes containing various functional ligands probably gives rise to the unique formation of the complexes having unprecedented or enhanced properties. Therefore, we have tried to investigate synthesis of group 10 metal pseudo-halogen complexes and their chemical reactivity toward organic unsaturated compounds. First, we here report synthesis of group 10 metal azides containing various phosphines or C~N donor ligands and their chemical properties toward organic isocyanides (C≡N-R) or isothiocyanate (R-N=C=S) to afford C-coordinated tetrazoles, carobodiimides (N=C=N-R), and S-coordinated tetrazoles, depending the supporting ligand. Second, we present Suzuki-Miyaura C-C coupling reactions catalyzed by various Pd pseudo-halogen compounds having functional ligands such as C~N donors or π-allyl ligands. Finally, we report the formation of novel macrocyclic complexes composed of five-membered palladacycle or platinacycle having a dimeric isocyanate unit as well as the catalytic cyclotrimerization of organic isocyanates (R-N=C=O).

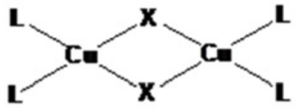
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR1-3**
발표분야: Recent Trends in Inorganic Chemistry I: Symposium for Senior Professors
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김영조

Crystal-to-Crystal Transformations and Luminescent Properties of Copper(I) Complexes

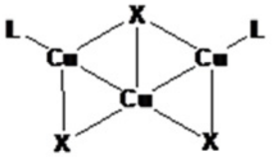
김진은

경상대학교 화학과

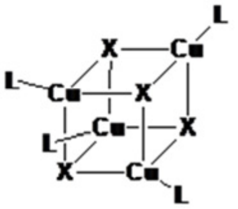
Recently, there has been considerable interest in the structural and photophysical properties of mono- and poly-nuclear complexes of transition metals ions (Cu(I), Ag(I), Au(I)) having the d^{10} electronic configuration. Cu(I) complexes exhibit a high structural diversity because of the relatively small energy difference between the various polymorphs under different synthetic conditions. Cu(I) complexes based on ligands with soft donor atoms such as aromatic N, S, and P show strong emission properties. Reversible/irreversible structural transformations and luminescence changes in these compounds as functions of temperature and solvent have been studied recently. These complexes that exhibit reversible modification of the emission wavelength in response to external stimuli are promising candidates for the development of smart photovoltaic materials, memory devices, or sensors. In this presentation, an overview of recent advances in the crystal-to-crystal transformations and luminescent properties of copper(I) complexes.



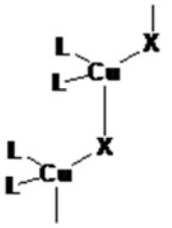
square dimer



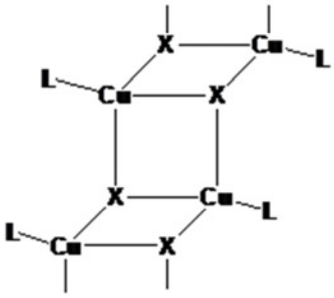
planar trimer



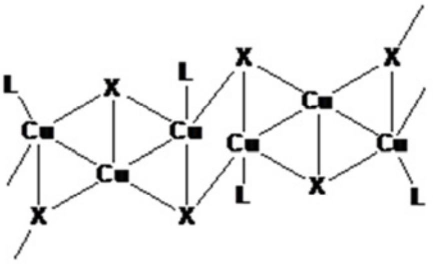
cubane tetramer



zigzag polymer



stair step tetramer



planar trimer stair step polymer

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR1-4**
발표분야: Recent Trends in Inorganic Chemistry I: Symposium for Senior Professors
발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 김영조

Single molecule picking and quantification of biomarkers with AFM

박준원

POSTECH 화학과

Self-assembly of dendrons provided nano-spacing between reactive functional groups on surface. The spacing guarantees the freedom of biological macromolecules so that their properties are close to that in solution in spite of the confinement in the two dimensional space. Such surface modification was integrated with atomic force microscopy (AFM) and the approach enabled new applications. For the DNA-DNA interaction, both binding and unbinding events were observed, and guaranteed single molecular interaction was a key advantage from the controlled surface. In particular, the mapping capability of AFM enabled us to see various biomarkers (DNA, mRNA, microRNA, antigen, and antibody) captured on surface. In particular, fabricating a tiny spot (a few microns in diameter) of the capture probe enhanced the detection limit dramatically. In this talk, both single molecule manipulation and quantification of biomarkers with AFM will be introduced.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR2-1**
발표분야: Recent Trends in Inorganic Chemistry Ⅱ: Metal–Organic Frameworks
발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 이창연

Metal-Organic Framework-Derived Functional Porous Metal Oxides, Carbon and their Composites

문회리

UNIST 화학과

Rational design of organic and metal building blocks has successfully enabled the genesis of variety of coordination polymers or metal-organic frameworks (MOFs) that are of fundamental scientific importance as well as provide a myriad of practical applications including catalysis. Our aim to design new MOFs is the utilization as ‘precursors’ to synthesize new nanostructured materials, which cannot be achieved by conventional synthetic methods. Since MOFs are composed of organic and inorganic part, well-tailored MOFs can be transformed to metallic/metal oxide nanomaterials or carbon-based materials under appropriate reaction conditions. To understand and develop this “transformation chemistry”, in-depth understanding of coordination chemistry is of crucial importance. In this talk, we present novel synthetic strategies that exploit a MOF-driven, self-templated route towards nanoporous metal oxides and graphitic carbon materials via thermolysis and their interesting applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR2-2**
발표분야: Recent Trends in Inorganic Chemistry Ⅱ: Metal–Organic Frameworks
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 이창연

Metal-Organic Frameworks for Industrially Important Gas Separations

배윤상

연세대학교 화공생명공학과

Metal-organic framework (MOF) is a new class of nanoporous materials, which have extremely high surface areas (~7000 m^2/g) and high porosity as well as well-defined pore size. The building-block synthesis approach creates the possibility to synthesize an almost unlimited number of structures and to tailor their pore sizes and functionalities in a precise way. Due to these interesting features, MOFs are considered as promising materials for various industrial applications, especially for various gas separations. This presentation introduces the recent studies on MOFs for industrially important gas separations such as Xe/Kr separation, SF_6/N_2 separation and olefin/paraffin separation. Material synthesis and characterizations, adsorption measurements, molecular modeling and process simulation techniques are combined to develop new MOFs for gas separations and to understand molecular-level adsorption behaviors in MOFs.*Acknowledgements*: This work was supported by the R&D Convergence Program of MSIP (Ministry of Science, ICT and Future Planning) and NST (National Research Council of Science & Technology) of the Republic of Korea (CRC-14-1-KRICT) and In-house Research and Development Program of the Korea Institute of Energy Research (KIER) (B6-2441).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR2-3**
발표분야: Recent Trends in Inorganic Chemistry Ⅱ: Metal−Organic Frameworks
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 서원석

MOFs-derived catalysts for organic and electrochemical reaction

이창연

인천대학교 에너지 화학공학과

Metal-organic frameworks (MOFs), consisting of organic building block and metal or metal-cluster secondary building unit (SBU), have emerged as a promising alternative to conventional porous materials due to their ultra-high surface area, structural diversity, controllable pore sizes and tailorable functionality. Distinct benefits of MOFs from other porous materials have led to tremendous potential applications such as gas and chemical storages, separations, sensor, light-harvester, drug delivery and catalysis. Among them MOF-based catalysis is one of the most widely demonstrated application. Organic functional group transformation, gas phase reaction and electrochemical reaction have been catalyzed with MOFs recently. Highly densed and homogeneously distributed metal site as well as nanoscopic reaction environment of MOFs are excellent benefits for catalysis applications. Herein, we will present the details of MOFs-derived carbon materials which were prepared by simple pyrolysis of various MOFs and their catalytic performance for organic and electrochemical reaction.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR2-4**
발표분야: Recent Trends in Inorganic Chemistry Ⅱ: Metal–Organic Frameworks
발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 서원석

Metal-organic framework based composited materials toward catalysis, sensing and switching applications

윤민영

가천대학교 글로벌캠퍼스 나노화학과

Metal-organic frameworks (MOFs), a series of coordination polymers with well-defined pores, have widely studied for various applications including gas storage/separation, catalysis, sensing, transport, and magnetism due to designability, tunability and functionalizability. Recent interests in multifunctional materials, however, triggered for the development of MOF based multifunctional materials. Several strategies have proposed; 1) incorporation of multiple ligand or metal nodes in the strut of MOFs, 2) incorporation of additional nanomaterials in the pores of MOFs, 3) conversion of MOFs by pyrolysis, and 4) mixing of nanomaterials by compositing. Among many kind of multifunctional MOFs synthesis strategies, pyrolysis and compositing of MOFs will be presented. Simple pyrolysis of MOFs allows preparation of a pure copper nanoparticle embedded porous carbon composite. The copper nanoparticles embedded composite demonstrated unique peroxidase like catalytic activity in glucose sensing. Due to the cooperative effect of uniformly distributed copper nanoparticles and hierarchical porosity of the composite, the material demonstrated one of be best glucose sensing sensitivities (3.2 x 10^{-7} M) as a colorimetric sensor. In addition, simple compositing of magnetic nanoparticles (such as Fe_3O_4)with MOFs allows switching of materials property by external magnetic field such as gas sorption properties. The switching efficiency of the composite was dependent on the external magnetic field. Furthermore, magnetic moment dependent switching study of the composite materials is now in progress. Therefore, cooperative behaviors or multifunctional behaviors of the composite materials will be useful for the development of efficient nanomaterial.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR2-5**
발표분야: Recent Trends in Inorganic Chemistry Ⅱ: Metal−Organic Frameworks
발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 서원석

Polymeric Metal-Organic Polyhedra: What are they and what are they good for

최원영

UNIST 화학과

Making hybrid materials based on Metal-Organic Polyhedra (MOPs) is quite limited possibly due to stability of MOPs and lack of synthetic protocol. In this presentation, a series of mechanically stable MOPs with permanent porosity are presented. Their metal joints are based on Zr clusters, similar to those found in well-established UiO-66. Utilizing these robust MOPS, we have further synthesized polymeric MOPs crosslinked by alkyl chain molecules. We will show similarities and differences between metal-organic frameworks and these new class of materials.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

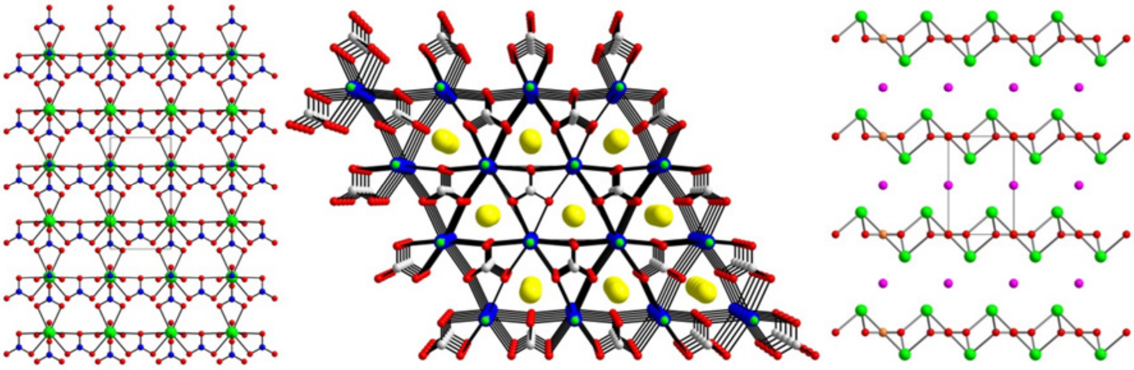
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR3-1**
발표분야: Recent Trends in Inorganic Chemistry Ⅲ: Organometallic Catalysis and Inorganic Materials
발표종류: 분과기념강연, 발표일시: 금 13:30, 좌장: 이강문

Nonlinear Optical (NLO) Materials Containing π-Delocalized Anionic Groups

옥강민[*] **Zouguohong**

중앙대학교 화학과

Nonlinear optical (NLO) materials have drawn enormous attentions attributable to their important applications in solid state lasers, optical communications, frequency conversions, and lithography. Although many efforts have been made to discover excellent NLO materials, it still remains challenging to design novel NLO materials exhibiting superb properties such as wide transparency windows for the high damage threshold, large second-harmonic generation (SHG) coefficients, good chemical stability, and moderate birefringence for the phase-matching condition. Among several noncentrosymmetric (NCS) chromophores, materials containing π-delocalized anionic groups such as NO_3^-, CO_3^{2-}, and BO_3^{3-} are of great current interest owing to their special applications to ultraviolet (UV) or deep UV-NLO materials. In this lecture, a series of meticulously designed novel polar noncentrosymmetric (NCS) materials with π-delocalized anioic groups are introduced. Structural determinations using single-crystal X-ray diffraction and the powder SHG measurements on the graded polycrystalline samples are presented. Structure-property relationships are elucidated from the solid-state structures and electronic structure calculations.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR3-2**
발표분야: Recent Trends in Inorganic Chemistry Ⅲ: Organometallic Catalysis and Inorganic Materials
발표종류: 분과기념강연, 발표일시: 금 13:50, 좌장: 이강문

Coordination Exchange at Open Metal Sites in MOFs

정낙천

DGIST 신물질과학과

Open metal site (OMS) on intersectional metal ion has shown considerable potential in its role for the applications in i.e., high ion transport and efficient gas adsorption. Thus, the activation of MOFs, the removal of solvent molecules (typically used in during the synthesis) from the OMSs has been thought as a prerequisite process for those applications. To date, several strategies for activating MOFs have been suggested: (i) thermal activation; (ii) freezing-drying; (iii) supercritical CO2 exchange; (iv) acid treatment. Among them, the thermal activation, which is normally performed by applying heat and vacuum, has been a unique way to remove the OMS-coordinated solvent molecule, whereas the other four methods are useful only for removing pore-filling solvents. Given that the high temperature (e.g., >150 C) can lead to structural damage to MOFs, conceivable low-temperature process will be a considerably promising way, compared to the cumbersome, pricey heat-and-vacuum technique.In this presentation, we will discuss how to control the activation condition for maintaining structural integrity during the activation process. As an example, I will show a new activation method, “chemical activation”, where methylene chloride (MC) plays a substantial role in removing both metal-coordinating and pore-filling solvents even at room-temperature. While MC treatment is surely a well-known method for replacing pore-filling solvent prior to thermal activation process in order to lower the activation temperature, the role of MC for breaking the metal-solvent coordination has never been demonstrated. We found that the chemical activation by MC arises via (i) replacement of pre-coordinated solvent by MC (the step before MC coordination) and (ii) spontaneous decoordination of MC (the step after MC coordination) with low activation energy which corresponds to room temperature. Also, we show that this low-temperature activation technique is more suitable for large-area MOF films.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR3-3**

발표분야: Recent Trends in Inorganic Chemistry Ⅲ: Organometallic Catalysis and Inorganic Materials

발표종류: 심포지엄, 발표일시: 금 14:10, 좌장: 박명환

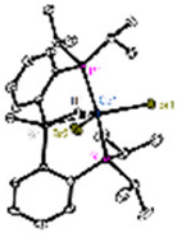
σ-Complexes of Cobalt and Copper

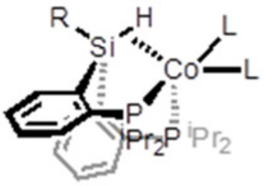
이윤호

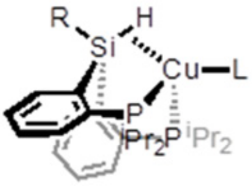
KAIST 화학과

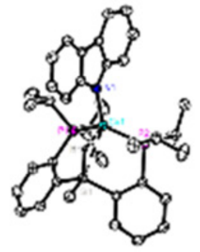
The binding of a Si–H bond to a single metal center is of particular interest. Understanding binding modes of a Si-H-M moiety is crucial in metal-catalyzed transformations involved in various hydrosilylation. Along with a well-known oxidative addition process of a Si-H bond, generation of a silyl metal species can occur via nonclassical σ-SiH interaction. To explore details of hydrosilylation mechanism, a Si-H bond was introduced to a series of divalent metal ions by preparing nickel and cobalt complexes supported by an anionic diphosphinosilyl $RSiP_2$ ligand ($RSiP_2 = RSiH[2\text{-}P\textit{i}Pr_2\text{-}C_6H_4]_2$; R = Me or Ph). While a clean conversion occurs in the reaction of a silane ligand with nickel(II) bromide, the formation of cobalt congeners $(MeSiP_2)CoBr$ reveals a low-temperature stable cobalt-SiH intermediate species $(MeSi^{H}P_2)CoBr_2$. Unusual reactivity of the green intermediate was carefully investigated by employing low-temperature UV-Vis and EPR spectroscopies. Using various tools including X-ray diffractions, ENDOR and high-level DFT calculations, the exact position of the hydrogen atom in the paramagnetic intermediate species was detected to reveal a highly unusual Co–H distance of ~1.53 Å. Surprisingly, we found evidence that the Si–H bond activation proceeds via deprotonation followed by Co–silyl coordination, rather than in the classical oxidative addition pathway. In fact, the same moiety was also introduced to a copper(I) ion to minimize geometry relaxation in metal-to-ligand charge transfer (MLCT) excited states by lifting the degeneracy of relevant Cu d-based orbitals. Such effect can be evaluated by studying copper emission property and ultimately utilized in developing efficient copper emitters. A series of corresponding cuprous complexes $(RSi^{H}P_2)Cu(Cbz^{R})$ were synthesized revealing unusual emission property exhibiting a blue/green emission band at λ_{max} = 474–513 nm with a high quantum efficiency (φ = 0.40–0.59) and a long lifetime of 15–23 μs. This emissive behavior contrasts with tetrahedral copper analogues, which do not display the blue emission due to a significant Jahn-Teller

distortion after the MLCT transition from nearly degenerate Cu d-based orbitals. Details of syntheses and photophysical properties of copper complexes will be discussed.









대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR3-4**

발표분야: Recent Trends in Inorganic Chemistry Ⅲ: Organometallic Catalysis and Inorganic Materials

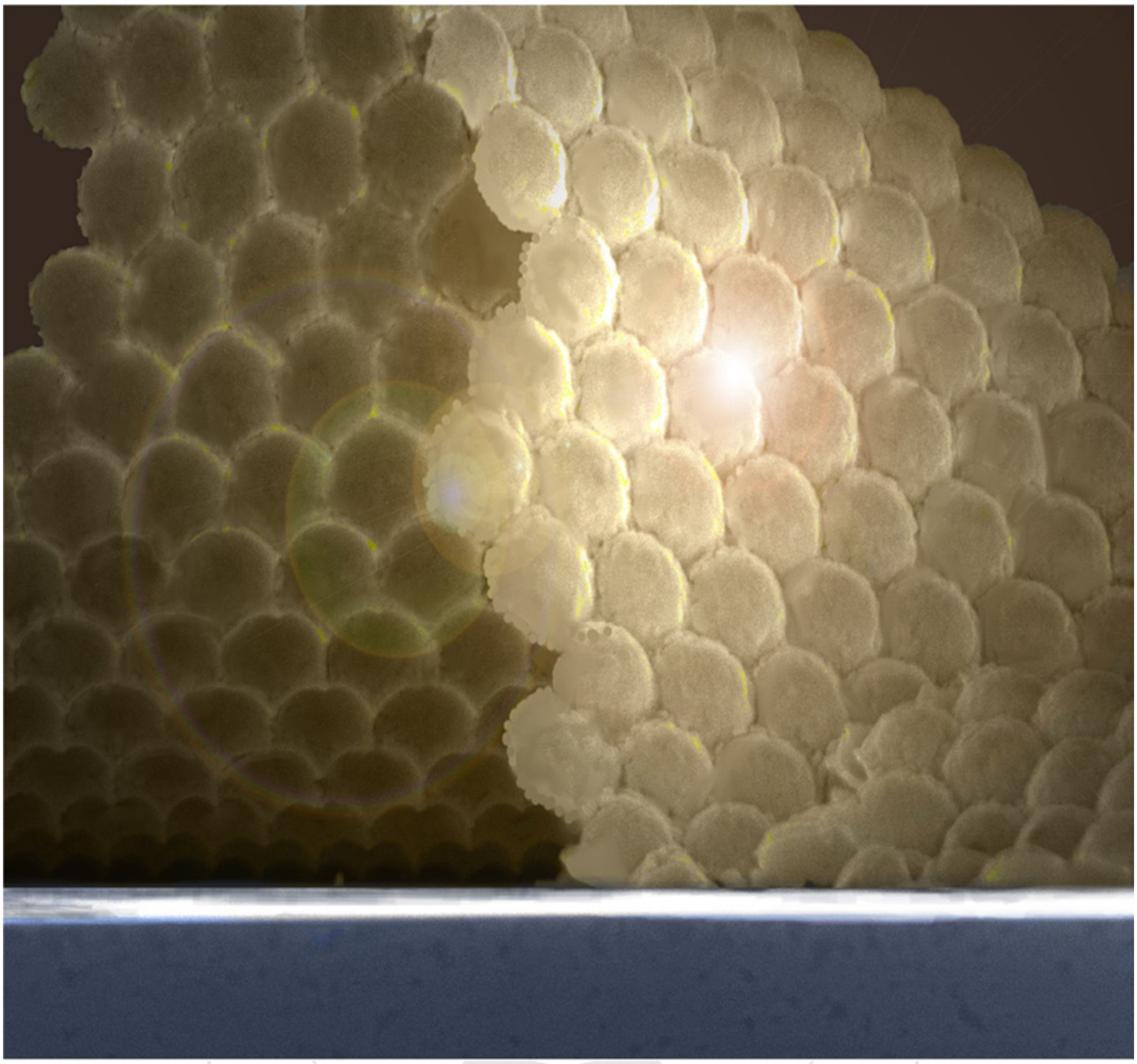
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 박명환

Fabrication of versatile metallic nanopatterns using anodized aluminum oxide templates and those usage for plasmonics and energy applications

이민형

경희대학교 응용화학과

Metallic nanopatterns are useful for various applications such as plasmonics, electronics, and photovoltaics. However, these applications are often limited by high-cost but low-throughput fabrication methods. In this talk, facile fabrication methods that can create long-range ordered metallic nanostructures over large-area with high controllability in geometries will be introduced. The fabricated metallic nanostructures exhibit interesting optical and electrical properties depending on those geometries. For example, hollow nanodomes and hierarchical nanopores in Au were fabricated which exhibits unique plasmonic resonances. Also, Cu meshes show specific selectivity in product of electrical CO_2 reduction depending on geometry.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR3-5**
발표분야: Recent Trends in Inorganic Chemistry Ⅲ: Organometallic Catalysis and Inorganic Materials
발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 박명환

The solution processed inorganic materials for large area electronics

김명길

중앙대학교 화학과

The recent developments of new electronic applications, such as flexible electronics, wearable electronics, and sensor arrays, requires innovative materials and processing strategy for high performance and low cost fabrications. Compared to conventional vacuum processing method, the solution processing of inorganic materials provide low cost and novel functionalities. Unfortunately, the relatively low performance and high processing temperature hinder the successful application of solution processing methods for next generation electronic applications. In this talk, I discuss the recent development of new soluble precursor for high performance electronic applications with low processing temperature.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR3-6**
발표분야: Recent Trends in Inorganic Chemistry Ⅲ: Organometallic Catalysis and Inorganic Materials
발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 박명환

Dioxygen Activation Beyond Metal-Oxo Species

조재홍

DGIST 신물질과학

Metalloenzymes activate dioxygen to carry out a variety of biological reactions. The dioxygen activation at the catalytic sites of the enzymes occurs through several steps including the binding of O2 at a reduced metal center, the generation of metal-superoxo and -peroxo species, and the O-O bond cleavage of metal-hydroperoxo complexes to form high-valent metal-oxo oxidants. Because these mononuclear metal-dioxygen (M-O2) adducts are implicated as key intermediates in dioxygen activation reactions catalyzed by metalloenzymes, studies of the structural and spectroscopic properties and reactivities of synthetic biomimetic analogues of these species have aided our understanding of their biological chemistry. In this presentation, we report the synthesis, structural and spectroscopic characterization, and reactivity studies of M-O2(H) complexes bearing tetraazamacrocyclic pyridinophane ligands. We have used various spectroscopic techniques, including UV-vis, EPR and resonance Raman spectroscopy, and density functional theory calculations to characterize several novel M-O2(H) complexes. Reactivity studies performed with the M-O2(H) complexes in oxidative nucleophilic and electrophilic reactions. Different steric properties of the supporting ligands control the reactivity of the intermediates. In addition, we investigate the reactivity comparison of M-O2 and -O2H species toward organic substrates.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS1-1**
발표분야: Machine Learning and Chemistry
발표종류: 분과기념강연, 발표일시: 목 13:00, 좌장: 은창선

Surface Analysis by Mass Spectrometry for Nano-Bio Applications

이태걸

한국표준과학연구원(KRISS) 미래융합기술부

Although the collisional cascade process in ToF-SIMS is unable to produce secondary ions with a molecular weight of over m/z 2,000 without the use of noble metals or special matrixes, time-of-flight secondary ion mass spectrometry (TOF-SIMS) imaging is a powerful technique for producing chemical images of small biomolecules (ex. metabolites, lipids, peptides) “as received” because of its high molecular specificity, high surface sensitivity, and submicron spatial resolution. For large biomolecules, 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.
For this talk, I will show that the label-free ToF-SIMS imaging technique can be a platform technology for characterization of organic-conjugated nanoparticles, disease diagnosis and drug screening. In addition, I will discuss the potential capability of Ar-cluster SIMS to study omics, particularly proteomics and lipidomics for brain studies.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS1-2**
발표분야: Machine Learning and Chemistry
발표종류: 심포지엄, 발표일시: 목 13:40, 좌장: 은창선

Illicit drug LC-MS/MS screening using machine learning and artificial intelligence approaches

오한빈

서강대학교 화학과

Phosphodiesterase 5-type (PDE-5) inhibitors and its analogues are known to be illegally added into dietary supplements. Regulating authorities of many countries have their own screening system to screen out those illicit drug use. In most cases, database-based LC-MS/MS screening system is widely used, but the ever-increasing modifications of the chemical structures of PDE-5 inhibitors and its analogues hamper the application of the database-based screening methods. In order to cope with the ever-changing modifications of the PDE-5 inhibitors and its analogues, construction of in-silico database is needed. For use of the in-silico database, predictions of the LC-MS/MS patterns and LC retention times are necessary. For this purpose, machine learning and artificial intelligence approaches can be adopted. In our studies, LC-MS/MS spectra of PDE-5 inhibitors and analogues plus other compounds are trained to classify LC-MS/MS spectra of unknown compounds under examination and furthermore LC retention times of newly added in-silico entities of PDE-5 inhibitors and analogues can be predicted with high accuracy.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS1-3**
발표분야: Machine Learning and Chemistry
발표종류: 심포지엄, 발표일시: 목 14:05, 좌장: 은창선

Development of New Genetic Algorithm and 3D Quantum QSAR for Predicting the Molecular Physicochemical Properties

박황서

세종대학교 바이오융합공학과

A major problem in molecular design concerns the accuracy in predicting the physicochemical properties of candidate molecules. We have had a particular interest in the development of computational methods for estimating the solvation free energy, protein-ligand binding affinity, and the toxicity of molecules due to the pharmaceutical importance. To obtain a proper solvation model, we established a solvation energy function based on the solvent-contact model, which involved the parameters for atomic volume, maximum atomic occupancy, and atomic solvation free energy with respect to varying atom types. These atomic parameters were then optimized with the standard genetic algorithm using the experimental solvation free energy data. The outperformances of this solvation model were verified in SAMPL4 and SAMPL5 blind prediction challenges for molecular hydration free energy and partition coefficient, respectively. New 3D quantum mechanical quantitative structure-activity relationship (Q-QSAR) model was developed using the electrostatic potentials calculated from the molecular orbitals as descriptor. The prediction accuracy of 3D Q-QSAR was then compared with that of classical comparative molecular field analysis (CoMFA) method. By virtue of using the more accurate molecular descriptors, the outperformances of 3D Q-QSAR over the CoMFA method were confirmed in predicting the molecular toxicities as well as in the protein-ligand binding affinities. 3D Q-QSAR method is thus anticipated to serve as a valuable computational tool for molecular design.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS1-4**
발표분야: Machine Learning and Chemistry
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 이명원

Machine learning approaches to the configuration energies and chemisorption models in solids

정유성

KAIST EEWS 대학원

Machine learning approaches are now beginning to be actively explored in theoretical chemistry, and in particular, perhaps as an important starting point, efficiently describing the energies of molecules have recently been proposed and shown reasonable performances. Yet, the need for the machine to eventually learn many-body effects as well as subtle correlations poses a significant challenge for these approaches to achieve high accuracy for general purposes. In this talk, we focus on the configuration energies of solids and some chemisorption models on them, and illustrate that the machine learning approaches can indeed be a useful alternative to the existing models to evaluate the latter energies. For both cases, we obtain mean absolute errors of 0.05-0.13 eV based on the artificial neural networks.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS1-5**
발표분야: Machine Learning and Chemistry
발표종류: 심포지엄, 발표일시: 목 15:05, 좌장: 이명원

QSPR modeling for screening high energy molecules(HEMs) using machine learning methods

이성광* 박한웅 김현정 이민지 이병훈 서현일[1] 조수경[2] 김한조[3] 윤정혁[4]

한남대학교 화학과 [1](주)퀀텀소프트 [2]국방과학연구소 4본부-2부 [3]CJ헬스케어 신약연구센터 [4](주)파로스아이비티 -

High energetic molecules (HEMs) are widely used for various civil, military and architecture applications. Generally, the promising HEMs should have the characteristics of enhanced detonation performance and low impact sensitivity. Removal of poor candidate HEMs before investing in synthesis and testing will go far toward developing the promising HEMs. Therefore, the importance of predictive modeling for searching potential HEMs has also increased as it minimizes extremely cost/time-consuming and risky step of synthesis as well as experiments of untested HEMs. The main parameters to evaluate the sensitivity and performance of HEMs are impact sensitivity, which expresses safe quality of HEMs to external stimuli, and detonation velocity or pressure, which were calculated from heat of formation and density by Kamlet-Jacobs equation. In this study, we will explain predictive QSPR modeling for screening insensitive HEMs, including representation of HEM structure, and supervised machine learning. The QSPR models were evaluated according to the OECD principles for QSAR/QSPR validation, and compliance with all five principles was established.Finally, we present newly developed softwares; that is, MS-HEMs 2 and PharosQSAR. MS-HEMs2 has been developed in response to need for information management and rapid prediction of HEMs properties. PharosQSAR is designed to build, utilize and import/export QSPR models. These softwares enables us to facilitate rational design of HEMs and to share QSAR/QSPR models was published in journal.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS1-6**
발표분야: Machine Learning and Chemistry
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 이명원

iQSAR : an interactive QSAR environment in IPython notebook Jupyter

김신영 조광휘*

숭실대학교 생명정보학과

iQSAR is a new Python/IPython utility designed specifically to be used for the construction of Quantitative Structure-Activity Relationships in a platform-independent manner. iQSAR modules allow one to quickly solve QSAR-specific problems interactively and create analyses that are reproducible by other researchers. While constructing QSAR analyses often warrants use of proprietary software which leaves the researcher dependent on the developers of QSAR and data analysis software, iQSAR seeks to allow the researcher to be in charge of tools for the QSAR process. With a flexible environment suited to quick iteration (similar to R or MATLAB), iQSAR modules may be used in any step in the QSAR construction process after descriptor selection. Particularly used in conjunction with IPython notebook, code and data can be published together and used as supplements to published material. A movement toward open-source and reproducible computing tools will allow the community to have a full understanding of the results published in a typical QSAR.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS2-1**

발표분야: Physical Chemistry of Biomolecules and Cells

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 허지영

Sequential Enzymatic Reactions and Electrostatic Channeling

은창선

한국외국어대학교 화학과

In cells, many enzyme-catalyzed reactions are coupled as a series of biochemical steps and thus, the reaction rate is dependent on the kinetics of intermediate reaction steps. In this work, we study the case of two coupled enzymatic reactions, where the product of the first reaction serves as the substrate of the second reaction. Specifically, we examine how the maximal rate of product generation in a series of sequential reactions is dependent on the enzyme distribution and the electrostatic composition of its participant enzymes and substrates. We further quantify the extent to which the electrostatic potential increases the efficiency of transferring substrate between enzymes, which supports the existence of electrostatic channeling observed in nature. We demonstrate the interplay of these concepts for the dihydrofolate reductase-thymidylate synthase (DHFR-TS) systems, whereby methylenetetrahydrofolate is converted via dihydrofolate to tetrahydrofolate. These findings shed light on the interplay of long-range interactions and enzyme distributions in coupled enzyme-catalyzed reactions, and their influence on signaling in biological systems.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS2-2**
발표분야: Physical Chemistry of Biomolecules and Cells
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 허지영

Highly Toxic and Stable Off-pathway Oligomerization of Islet Amyloid Polypeptide Mediated by Cu(II)

김준곤

고려대학교 화학과

Human islet amyloid polypeptide (hIAPP) is an amyloidogenic protein associated with the pathogenesis of type II diabetes mellitus (T2DM). The toxicity of hIAPP amyloidosis is suggested to be due to oligomeric intermediates rather than insoluble fibrils; however, structural information about these oliogmers is quite limited and therefore elucidation of the structure-toxicity relationship of hIAPP remains elusive. In this presentation, a direct observation of the toxic oligomers of hIAPP, produced through a newly discovered Cu(II)-mediated off-pathway aggregation process, is discussed as well as structural data obtained from various biophysical methods in conjunction with theoretical modeling. The Cu(II)-triggered assemblies of hIAPP oligomers show a highly symmetric flattened cylinder shape, formed via isotraopic aggregations, and display noticeable toxicity toward pancreatic beta-cells. Overall, our studies demonstrate an off-pathway aggregation process for the formation of toxic hIAPP oligomers, which will provide a foundation for developing therapeutic strategies against T2DM.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS2-3**
발표분야: Physical Chemistry of Biomolecules and Cells
발표종류: 심포지엄, 발표일시: 금 09:50, 좌장: 허지영

Network analysis on the conformational change of c-Src tyrosine kinase employing molecular dynamics simulation

윤현정 박선주[1,*] <u>우상욱</u>[*]

부경대학교 물리학과 [1]부경대학교 화학과

A non-receptor Src-family protein tyrosine kinases (SFKs) play a critical role in cell growth, differentiation, and various metabolism by controlling cell signal. The regulation of cell signaling by SFKs is mediated by the conformational activation/inactivation of the tyrosine kinase. We investigated the conformational change of c-Src, one of the member of SFKs, from the inactive form (PDB id: 2SRC) to the active form (PDB id: 1Y57) employing targeted molecular dynamics (TMD) simulation. Based on the network analysis, we proposed allosteric pathway for the conformational change of the c-Src tyrosine kinase.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS2-4**
발표분야: Physical Chemistry of Biomolecules and Cells
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 이강택

Probing and manipulating cellular behaviors by silicon nanowire arrays

<u>김소연</u>

한국과학기술연구원(KIST) 의공학연구소

Intensive studies have illustrated the broad implications of vertical nanowire (NW) arrays for manipulating mammalian cells in vitro. As such examples, a newly developed approach for probing protein interactions in living cells will be presented. In addition, I will describe how NW arrays can actively control cell-to-substrate interaction and induce the spontaneous formation of induced pluripotent stem cell derived spherical colonies with unlimited self-renewal and differentiation potentials.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS2-5**

발표분야: Physical Chemistry of Biomolecules and Cells

발표종류: 심포지엄, 발표일시: 금 10:50, 좌장: 이강택

Charged biomolecules in aqueous cell

조용석

기초과학연구원 CSLM

The presence of polar water in cell reduces ionization barrier significantly so that most biological molecules are charged either locally or globally. For this reason, the charge interaction is one of the most important long range interaction governing the behavior of these molecules. Recently, there have been intensive studies on the electrostatics of biological system in order to understand its anomalous behaviors which are originated from the inhomogeneity in electrostatic field, and explicit water dependence (specific ion effect). Some examples are attraction between like charges, repulsion between opposite charges, charge inversion, charge renormalization, phase separations of complex polyelectrolyte solutions, Hofmeister series, etc. Conventional theoretical approaches based on mean field theory often fail to explain these phenomena. Hierarchical structure and the mesoscopic nature are essential hurdles to understand these systems. In this talk, I will highlight theoretical and computational efforts to study the electrostatics of biological molecules.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS3-1**
발표분야: Recent Physical Chemistry Studies on Nanomaterials
발표종류: 분과기념강연, 발표일시: 금 13:20, 좌장: 권찬호

Controlled Assembly of Nanoparticles for Plasmon Coupling Studies

윤상운

중앙대학교 화학과

The assembly of noble metal nanoparticles offers an appealing means to control and enhance the plasmonic properties of nanostructures. Despite their great advantages, however, making nanoassemblies in a controlled fashion with high efficiency remains challenging. In this talk, I will present our efforts to assemble nanoparticles into various structures with high yields, including core-satellites, sphere dimers, and sphere-cube dimers.[1–3] The interparticle distance (d) in these assemblies is finely tuned at the molecular level using self-assembled monolayers of alkanedithiol linkers. The controlled interparticle distance and ultrahigh purity of the prepared nanoassemblies allow us to investigate the plasmon coupling between the nanoparticles as a function of the gap distance. We find that the plasmon coupling follows the classical electromagnetic model when the nanoparticles are far apart ($d > 1$ nm); however, quantum tunneling effects play a significant role in the plasmonic response of nanoassemblies in the subnanometer gap region.[1,2,4] I will also briefly introduce our recent attempts to control the interparticle distance continuously using photooxidative desorption of linkers.[5] At the end of the talk, I will discuss the future direction of our research.

[1]Cha, H.; Yoon, J. H.; Yoon, S. *ACS Nano* **2014**, *8*, 8554.
[2]Yoon, J. H.; Lim, J.; Yoon, S. *ACS Nano* **2012**, *6*, 7199.
[3]Lee, D.; Yoon, S. *J. Phys. Chem. C* **2015**, *119*, 7873.
[4]Yoon, J. H.; Zhou, Y.; Blaber, M. G.; Schatz, G. C.; Yoon, S. *J. Phys. Chem. Lett.* **2013**, *4*, 1371.
[5]Jung, H.; Cha, H.; Lee, D.; Yoon, S. *ACS Nano* **2015**, *9*, 12292.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS3-2**
발표분야: Recent Physical Chemistry Studies on Nanomaterials
발표종류: 심포지엄, 발표일시: 금 14:00, 좌장: 권찬호

Unusual Light Emission from/on Graphene

전석우

KAIST 신소재공학과

Graphene quantum dots (GQDs), simply making graphene typically under 10 nm, and the change of emission behavior from known fluorescents on graphene draws huge interest for potential applications to display, lighting, and optoelectronic devices. GQD could be a new class of optical material with useful properties of tunable luminescence, superior photo-stability, and chemical resistance. Here, we demonstrate the first GQD light-emitting diodes (GQD-LEDs) with electroluminescence that exceeds 1,000 cd/m2. The GQD-LEDs are possible due to our simple synthesis method to create high-quality GQDs with minimal, or controlled, oxidation such that high quantum yields (~4.6%) are guaranteed. The GQDs are synthesized by the solvothermal formation of graphite intercalation compounds (GICs) between graphite powder and sodium potassium tartrate. The proposed method is cost-effective, eco-friendly, and can easily be scaled up, as it allows the direct fabrication of GQDs using water without a surfactant or chemical solvent. The GQD-LEDs, in which GQDs are incorporated into polymeric host layers in a multilayer electroluminescent (EL) device, irradiate blue (~400 nm) emission. Besides the direct emission from graphene, when conjugated fluorescent materials such as porphyrin interact with the conjugated plane of graphene, interesting peak shifts and emission enhancement from the fluorescent materials are observed. The demonstration of an optical transition of PtOEP, deposited on graphene, from triplet to singlet and strong PL enhancement will show the possibility of using graphene as new platform to modulate emission behaviors from fluorescent materials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS3-3**
발표분야: Recent Physical Chemistry Studies on Nanomaterials
발표종류: 심포지엄, 발표일시: 금 14:25, 좌장: 채원식

Beneficial Effects of Water in the Hot-injection Synthesis of InP/ZnS Core-Shell Quantum Dots

이종수

DGIST 에너지시스템공학

Nanoparticles of different metals, semiconductors and magnetic materials can self-assemble from colloidal solutions into long range ordered periodic structures (superlattices). Colloidal nanocrystals are considered promising building blocks for electronic and optoelectronic devices. In this presentation, I will explain that the presence of a small amount of water as an impurity during the hot-injection synthesis can significantly decrease the emission lines full width at half-maximum (FWHM) and improve the quantum yield (QY) of InP/ZnS quantum dots (QDs). By utilizing the water present in the indium precursor and solvent, we obtained InP/ZnS QDs emitting around 530 nm with a FWHM as narrow as 46 nm and a QY up to 45%. Without water, the synthesized QDs have emission around 625 nm with a FWHM of 66 nm and a QY of about 33%. As an example of their application in light-emitting diodes (LEDs), the green and red InP/ZnS QDs are combined with a blue LED chip to produce white light.
I will also show an efficient halide exchange reaction in cesium lead halide perovskite nanocrystals. The green light emitting CsPbBr3 nanocrystals can be tuned to emit over the entire visible spectral region (425~655 nm) by reacting with different concentrations of I or Cl precursors. The halide exchange reactions readily take place at room temperature and completed within seconds. A good photoresponsive behavior is observed for the $CsPbI_3$ NCs films, indicating their potential application in optoelectronic devices.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS3-4**
발표분야: Recent Physical Chemistry Studies on Nanomaterials
발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 채원식

Interface chemistry of colloidal quantum dots for display applications

고원규

삼성종합기술원 Device Lab

Colloidal quantum dots (QDs) have great potential in conventional display applications of light emitting diodes (LEDs) and lasers, as well as new area of photonic applications such as single photon emitters in quantum cryptography and communication. While there have been extensive research and development of colloidal QDs in display applications from understanding carrier dynamics to realizing electroluminescence devices and QD-based ultra high density TV, intrinsic challenge of QD application is still remained in engineering interface chemistry of QDs. As an individual, single dot spectroscopy is useful in understanding the role of interface in multi-shell QD structures. Cadmium selenide and indium phosphide-based QDs will be discussed to compare their probability density plots and Auger ionization efficiencies determined by analyzing their photoluminescence blinking dynamics. As a multi-component solid state device, we will discuss the critical role of interfaces in QD LEDs using spectroscopy and electrochemistry studies. These results suggest that the interface of QDs is closely associated with their charge transfer and radiative process, providing insight into the development of highly efficient QD-based display applications.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL1-5**

발표분야: Recent Trends in Analytical Chemistry I: Elemental and Environmental Analysis

발표종류: 분과기념강연, 발표일시: 목 15:00, 좌장: 김정권

Quadrupole nuclear magnetic resonance spectroscopic studies of various solid-state materials

이영일

울산대학교 화학과

Solid-state NMR spectroscopy is a powerful technique to understand local environment of various materials having quadrupole nuclei (I > 1/2), such as 7Li, 11B, 14N, 27Al, 59Co, 79,81Br, 93Nb, etc., To observe these quadrupole nuclei with NMR, specific techniques are required depending on nuclear species having quadrupolar effect and state of materials having different local structure. My presentation will begin to introduce my Ph.D thesis, which include “93Nb field sweep NMR spectroscopy with superconducting magnet”, “11B imaging with field-cycling NMR as a line narrowing technique”, “Field cycling 14N NQR imaging with spatial and frequency resolution”, and "Pulsed 81Br NQR spectroscopy of brominated flame retardants and associated polymer blends". Also, introduction of solid-state NMR spectroscopic studies with various quadrupole nuclei, such as 7Li, 27Al, and 59Co, to investigate local structure of cathode materials for lithium ion battery will be dealt. At last, development of new synthetic method and investigation of alternative cathode materials by cation and anion substitution in various structured materials will be also introduced.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1-1**
발표분야: Recent Trends in Analytical Chemistry I: Elemental and Environmental Analysis
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 박종호

The last frontier of elemental analysis: the persistent battle against small measurement biases

임용현

한국표준과학연구원(KRISS) 무기분석표준센터

As a national metrology institute, KRISS has established robust SI-traceable analytical methods to characterize elemental contents in candidate reference materials. Isotope dilution (ID) inductively coupled plasma-mass spectrometry (ICP-MS) and neutron activation analysis (NAA) are two examples of well-established methods for elemental analysis in complex sample matrices. Although they are even regarded as potential primary methods due to their robustness and SI-traceability, the analysis results often suffer from unexpected biases depending on analytes and sample matrices. In the present talk, some examples of our continuing fights against small, but not negligible, measurement biases will be illustrated. It includes the importance of oxidation state equilibration and control of spectral/non-spectral interferences in the area of ID ICP-MS. Recent development of an exact matrix matching ICP-optical emission spectroscopy (OES) as an additional potential primary method of elemental analysis will be also presented.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1-2**
발표분야: Recent Trends in Analytical Chemistry I: Elemental and Environmental Analysis
발표종류: 심포지엄, 발표일시: 목 13:50, 좌장: 박종호

Recent efforts for high-performed bulk analysis techniques of U and Pu at ultra-trace levels in environmental samples with MC-ICP-MS

임상호[*] 한선호[1] 송규석

한국원자력연구원 원자력화학연구부 [1]한국원자력연구원 분석화학실

Improved chemical procedures based on extraction chromatography, high-performed mass analysis technique with MC-ICP-MS (NEPTUNE Plus, Thermo Scientific, Germany) and systematic evaluations of measurement uncertainties of U and Pu analysis at ultra-trace levels in environmetal samples are presented. The major improvements of chemical procedures in this study were the chemical pre-treatment for complete acid digestion of target samples and chemical separation scheme with a single column system using UTEVA resin for increasing recovery yield of Pu isotopes. To improve signal sensitivities, reduce hydride formation and reduce long-term signal fluctuations, a desolvating nebulizer system (Aridus II, CETAC, USA) and a fine tunable peristaltic pump were adopted in the sample introduction system of MC-ICP-MS. In addition, we systematically evaluated the combined uncertainties of potential uncertainty factors during the overall chemical procedures to examine the reliability of analytical results. Finally, the quantification and isotopic ratio analysis of U and Pu were performed with the simulated swipe samples containing U and Pu standard materials to validate the analytical performance of improved bulk analysis techniques in this study. The anlytical results of the simulated swipe samples were in good agreement with the certified values, based on the measurement quality goals for the analysis of bulk environmental samples recommended by the International Atomic Energy Agency (IAEA)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL1-3**

발표분야: Recent Trends in Analytical Chemistry I: Elemental and Environmental Analysis

발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 박종호

Determination of inorganic arsenic by ion chromatography coupled with inductively coupled plasma mass spectrometry

남상호

목포대학교 화학과

Chemical transformation of arsenic element can result in various chemical forms that differ considerably in properties. The toxic and biological effects of arsenic depend on the different chemical species in a sample. This study focus on the development of standardized analytical method of inorganic arsenic species in various samples. The developed method for the quantitative determination of arsenic species included the selective extraction method, the optimization of the separation and detection method and all the important instrumental and methodological parameters. The prevention of loss and transformation of arsenic species was confirmed with the developed extraction and analytical method.Arsenic species were determined in rice that was produced in Korea, and the surrounding soil and water were analyzed to identify the source of inorganic arsenics. In a rice, the main arsenic species was As (III), and its concentration range was from 8 to 65 μg/kg. The concentrations of As (V) in a rice were in the range of 1.4 - 6.8 μg/kg. The major arsenic species was As (V) in paddy soil, and its concentration range was from 0.5 to 165 mg/kg. The concentrations of As (III) in paddy soils were in the range of 0.3 - 8.6 mg/kg. Only the inorganic arsenic species were in pore water samples. The organic arsenic species did not exist in any sample.The concentration of As (V) is much higher than that of As (III) in paddy soil, but the concentrations of As (III) in rice and pore water were higher than that of As (V). It was described that the mobility and uptake of arsenic relyed on the arsenic species. The mobility and uptake rate of As (III) were higher than that of As(V). The high content of arsenic species in paddy soil were closely related with the total concentration of arsenic species in rice.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1-4**
발표분야: Recent Trends in Analytical Chemistry I: Elemental and Environmental Analysis
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 김정권

Pb concentrations and the Pb isotope record in northwest Greenland snow

강정호

한국해양과학기술원 부설 극지연구소 극지고환경연구부

We present lead (Pb) concentrations and Pb isotope ratios from northwest Greenland snow pit samples covering a six-year period, from spring 2003 to early summer 2009. Pb concentrations ranged widely, from 2.7 pg g–1 to 99.7 pg g–1, with a mean concentration of 21.6 pg g–1; these values are statistically slightly higher than values recorded for 1991−1995. Pb concentrations exhibit seasonal spikes in winter−spring layers. Crustal Pb enrichment factors (EF) suggest that the snow pit is highly enriched with Pb of predominantly anthropogenic origin, with EF values inversely correlated with Pb concentrations. The 206Pb/207Pb isotope ratio of our samples ranged from 1.144−1.169, indicating relatively large differences between less radiogenic Eurasian-type and more radiogenic Canadian-type signatures, suggesting several potential source areas of Pb reaching northwest Greenland. Abrupt changes in Pb concentrations and Pb isotope ratios were observed and related to seasonal shifts in source regions of aerosol transport. The 206Pb/207Pb isotope ratio increased steadily between 2003 and 2009. The similarity in isotope ratios between our samples and Chinese urban aerosols suggest a relatively high and steadily increasing contribution of Chinese Pb to northwest Greenland snow.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2-5**

발표분야: Recent Trends in Analytical Chemistry Ⅱ: Analytical Chemistry in Microsystems

발표종류: 분과기념강연, 발표일시: 금 15:00, 좌장: 강덕진

MALDI TOF Mass Spectrometer: Development of an analytical instrument and Business as a medical instrument. MALDI TOF 질량 분석기: 분석기기에서 진단기기로, 개발에서 사업화까지

김양선

ASTA(주) 연구소

MALDI-TOF MS, matrix-assisted laser desorption-ionization -time-of-flight mass spectrometer has been used for the analysis of biomolecules (biopolymers such as DNA, proteins, peptides and sugars) and large organic molecules. It was named by Franz Hillenkamp and Michael Karas in 1985, and Coichi Tanaka received one-quarter of the 2002 Nobel Prize in Chemistry for demonstrating that, with the proper combination of laser wavelength and matrix, a protein can be ionized in 1987. The high throughput and high speed of MALDI TOF technique provide an accurate and inexpensive tool for clinical application. In this seminar, critical points to complete a commercial mass spectrometer, especially as a medical system starting from development of an analytical 'Time of flight mass spectrometer' will be presented. Recent clinical applications using MALDI TOF MS which is officially approved or under being developed will be introduced.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2-1**

발표분야: Recent Trends in Analytical Chemistry Ⅱ: Analytical Chemistry in Microsystems

발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 조건

Application of SERS-based Microfluidic Platform for Early Disease Diagnosis

주재범

한양대학교 생명나노공학과

We report a novel SERS-based microfluidic platform for the highly sensitive biomarker detection. In this presentation, we report the development of a programmable and fully automatic SERS-based microfluidic sensor that integrates a microfluidic device with a nanoparticle-based Raman detection platform. This device provides a convenient and reproducible immunoassay tool for various biomarkers. The utility of this device is demonstrated by the quantitative immunoassays of various intractable disease biomarkers. Our proposed biosensor platform has many advantages over other immunoassay methods such as good reproducibility, low limits of detection and fast assay times. The tedious manual dilution process of repetitive pipetting and inaccurate dilution is also eliminated with this process because various concentrations of biomarker are automatically generated by microfluidic gradient generators with mixing stages. The total assay time from serial dilution to detection takes less than 30 min because all of the experimental conditions for the formation and detection of immunocomplexes can be automatically controlled inside the exquisitely designed microfluidic channel. Thus, this novel SERS-based microfluidic device is expected to be a powerful clinical tool for early disease diagnosis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2-2**
발표분야: Recent Trends in Analytical Chemistry Ⅱ: Analytical Chemistry in Microsystems
발표종류: 심포지엄, 발표일시: 금 13:50, 좌장: 조건

Miniaturized systems for Alzheimer's disease: disease model and diagnostics

<u>김정아</u>

한국기초과학지원연구원 생의학오믹스연구팀

Alzheimer′s disease (AD) is a chronic, neurodegenerative disorder which is normally accompanied by pathologic hallmarks such as accumulation of extracellular amyloid plaques and intracellular neurofibrillary tangles. As the prevalence of Alzheimer's disease is expected to rise with the aging of the population, urgency for developing new treatment has been increased. For this research purpose, the decisive disease model of AD and its diagnosis tool is necessary. Here, we present two different approaches, relying on miniaturized systems, aiming at development of in vitro disease model and diagnostic system for AD. Firstly, we present the engineered three-dimensional (3D) in vitro brain neurovascular unit using miniaturized devices based on 3D printing and microfluidic techniques. The brain microvasculature model in vitro was developed for recreating the 3D neurovascular microenvironment, culturing the multiple cell types, and optimizing the differences in the media compositions that support these different types of cells. Secondly, we propose the miniaturized system for the quantification of oligomeric Aβ for AD diagnosis. This micro-pillar-embedded microfluidic chip simplified the complicated ELISA procedure and achieved high sensitivity. We also demonstrated that this can be utilized for the general ELISA assay, and it is expected to be the point-of-care testing platform with simple automation instruments in a rapid, easy-to-use, cost-effective way. Only 4 μg of magnetic beads were used in a chamber, and, consequently, a small amount of antibody was required for the AD diagnosis (10–30 ng of antibody per single assay). Furthermore, the assay time was reduced significantly to 40 min, including incubation. Overall, micro-and nano-techniques can serve as useful tools not only for fundamental studies associated with AD in physiological and pathological settings but also its clinical diagnosis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2-3**
발표분야: Recent Trends in Analytical Chemistry Ⅱ: Analytical Chemistry in Microsystems
발표종류: 심포지엄, 발표일시: 금 14:10, 좌장: 조건

Toward Atomically-Controlled Dendrimer-Encapsulated Nanoparticles: Synthesis and Useful Properties in Analytical Chemistry

김주훈

경희대학교 화학과

Here, we report on the synthesis of dendrimer-encapsulated nanoparticles (DENs) and their useful properties for analytical applications. Specifically, we synthesized Pt DENs containing an average of 55 Pt atoms using amine-terminated 4th-generation polyamidoamine (PAMAM) dendrimers, which we denote as G4-NH2(Pt55). The synthesized G4-NH2(Pt55) exhibited peroxidase-mimetic activity, superior or at least comparable to that of natural peroxidase enzymes such as horse radish peroxidase (HRP), and thus could be utilized as peroxidase-mimetic labels for sensitive colorimetric assays [1]. In addition, we synthesized Pt DENs using amine-terminated nth generation PAMAM (Gn-NH2, n = 6 and 4) dendrimers. The synthesized Pt DENs showed different sizes over the range of 1-3 nm, but were fairly uniform and monodispersed in size with subnanometer accuracy. Interestingly, we found the size-dependent catalytic activity of the Pt DENs having well-defined sizes with subnanometer accuracy for the enhanced chemiluminescence of the luminol/H2O2 system. We demonstrated the analytical versatility of the Pt DEN-catalyzed generation of chemiluminescence in oxidase-based analyses toward various oxidase substrates including choline, glucose, and cholesterol [2]. Finally, we also describe briefly how the Pt DENs can be utilized for sensitive electrochemiluminescence-based analyses [3]. References[1] Youngwon Ju and Joohoon Kim, Chem. Commun., 2015, 51, 13752-13755.[2] Hyojung Lim, Youngwon Ju, and Joohoon Kim, Anal. Chem., 2016, 88, 4751-4758.[3] Jihye Kwon, Seo Kyoung Park, Yongwoon Lee, Je Seung Lee, and Joohoon Kim, Biosens. Bioelectron., 2016, In press.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2-4**
발표분야: Recent Trends in Analytical Chemistry Ⅱ: Analytical Chemistry in Microsystems
발표종류: 심포지엄, 발표일시: 금 14:40, 좌장: 강덕진

irus based novel Colorimetric Sensor for Cancer Cell Detection

오진우

부산대학교 나노소재공학과

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

References

[1] W.-J. Chung, J.-W. Oh et al. *Nature* 478, 364 (2011).
[2] J.-W. Oh et al. *Nature Comm.* 5, 3043 (2014)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO1-1**
발표분야: Biochemistry of Proteostasis
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 김동은

Regulation of Proteotoxic Protein Homeostasis through the Proteasome

이민재

서울대학교 의과대학 생화학교실

Rates of proteolysis are a function of cell's physiological state and are controlled differentially for individual proteins, affecting a variety of regulatory pathways both in normal and pathological conditions. The proteasome is responsible for the degradation of most regulatory proteins in eukaryotes, where substrates were marked for degradation by the attachment of polyubiquitin chains. As our knowledge of biological processes in the system has grown for the last 30 years, so have the ties between the system and various human diseases including cancers, metabolic diseases, and neurodegenerative diseases. In this presentation, I intend to provide an example of studies which were involved in regulation of proteasome activity through small-molecule activators, direct delivery of exogenous proteasome, and structural modifications. These data demonstrate that 1) proteasome manipulation is possible and tolerable to cell, 2) understanding the pathological changes of proteostasis during the progression of disease is important, and 3) fine tuning of proteasome activity may function to be as a precision medicine.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO1-2**
발표분야: Biochemistry of Proteostasis
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 김동은

Ubiquitin E3 ligase STUB1-mediated proteolysis of tissue glutaminase 2 negatively affects tumor progression and angiogenesis in renal cancer

정광철

연세대학교 시스템생물학과

The multifunctional enzyme tissue glutaminase 2 (or transglutaminase 2, TG2) primarily catalyzes cross-linking reactions of proteins via (γ-glutamyl) lysine bonds. Several recent findings indicate that altered regulation of intracellular TG2 levels affects renal cancer. Elevated TG2 expression is observed in renal cancer. However, the molecular mechanism underlying TG2 degradation is not completely understood. STIP1 homology and U-Box containing protein 1 (STUB1; also known as carboxyl-terminus of Hsp70-interacting protein, CHIP) functions as an ubiquitin E3 ligase. Previous studies reveal that STUB1 deficiency mice displayed a reduced life span with accelerated aging in kidney tissues. Here we show that STUB1 promotes poly-ubiquitination of TG2 and its subsequent proteasomal degradation. In addition, TG2 upregulation contributes to enhanced kidney tumorigenesis. Furthermore, STUB1-mediated TG2 downregulation is critical for the suppression of kidney tumor growth and angiogenesis. Notably, our findings are further supported by decreased STUB1 expression in human renal cancer tissues and renal cancer cells. The present work reveals that STUB1-mediated TG2 ubiquitination and proteasomal degradation represent a novel regulatory mechanism that controls intracellular TG2 levels. Alterations in this pathway result in TG2 hyper-expression and consequently contribute to renal cancer.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO1-3**
발표분야: Biochemistry of Proteostasis
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김동은

A new strategy for inhibiting ubiquitin pathway using ubiquitin binding small molecules

김경규

성균관대학교 의학과

The ubiquitin pathway plays a critical role in regulating diverse biological processes, and its dysregulation is associated with various diseases. Therefore, it is important to have a tool to control ubiquitin pathway for better understanding this pathway as well as developing therapeutics against relevant diseases. We found that sulfonated aryl diazo compounds could inhibit the ubiquitin processing enzymes involved in ubiquitination and deubiquitination, and cell surface receptor that recognizes ubiquitin as a ligand. NMR mapping, docking and molecular dynamics simulations reveal that these compounds block interactions between ubiquitin and cognate proteins by direct binding to the β-groove, a major interacting surfaces of ubiquitin. Furthermore, we found that cellular localization of compounds varies depending on the overall charges, and thus intracellular or extracellular ubiquitin-protein interactions can be controlled using the location specific inhibitors. Eventually, we demonstrated that these ubiquitin binding chemicals can effectively suppress the cancer progress, suggesting chemical-mediated inhibition of ubiquitin binding can be used for cancer therapy. Our results suggest that ubiquitin binding molecules can be developed as inhibitors of ubiquitin pathways, which have the value in not only unveiling the biological role of ubiquitin but also treating related diseases.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO1-4**

발표분야: Biochemistry of Proteostasis

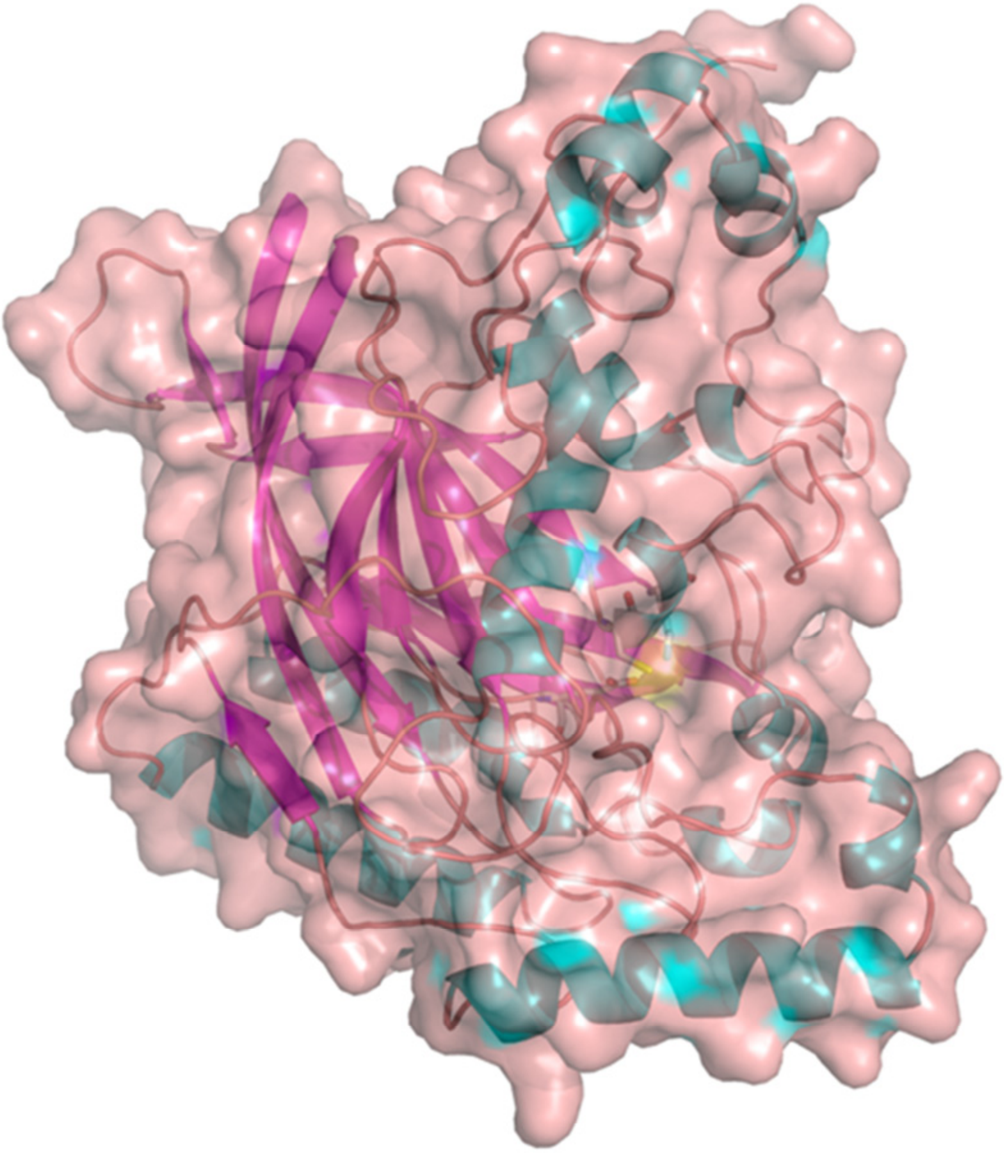
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 김동은

Structural basis for dual specificity of yeast N-terminal amidase in the N-end rule pathway

송현규

고려대학교 생명과학부

The first hierarchical step of the N-end rule pathway is deamination of N-terminal glutamine and asparagine residues to glutamic and aspartic acids, respectively. These reactions are catalyzed by the N-terminal amidase Nta1 in fungi such as Saccharomyces cerevisiae, and by the enzymes glutamine-specific Ntaq1 and asparagine-specific Ntan1 in mammals. To investigate the dual specificity of yeast Nta1 (yNta1) and the importance of the second-position residue of tertiary-destabilizing N-degron, crystal structures of yNta1 in the apo state and in complex with various N-degron peptides were determined. Both the Asn-peptide and Gln-peptide fitted well into the hollow active site pocket, and catalytic triads were located deeper inside the active site, leading to hydrogen bonds between N-degron peptides and hydrophobic peripheral regions of the pocket. Key determinants for substrate recognition were then clearly identified and confirmed using structure-based mutagenesis. Finally, binding constants of yNta1 and its mutants were measured, and also the enzyme kinetic parameters KM, and kcat for each peptide type were calculated. Taken together, the present data elucidate crucial mechanisms in the first step of the N-end rule pathway.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO1-5**
발표분야: Biochemistry of Proteostasis
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 김동은

Autophagic regulation of ALS-linked stress granule-associated aggregates

이진아

한남대학교 생명시스템과학과

Abnormal accumulation of cytosolic aggregates or inclusion bodies is a hallmark of several neurodegenerative diseases. Many common or specific molecular components such as ubiqutin, α-synulcein, TDP-43, or tau in neuronal cytosolic inclusion bodies have been identified as being associated with cellular pathogenic mechanisms of disease. Recently, stress granule (SG) marker proteins such as PABP and G3BP were found in cytosolic inclusion bodies of patients with frontotemporal lobar dementia (FTLD), Alzheimer's disease (AD), or amyotrophic lateral sclerosis (ALS), suggesting that inappropriate SG dynamics contributes to pathogenic mechanisms. However, the role of autophagy in regulation of disease associated stress granules (SGs) and aggregates remains unclear. We found that the ALS-linked FUS(R521C) or FUS(H517Q) mutation causes accumulation of FUS-positive SGs under oxidative stress, leading to disruption of release of FUS from SGs in cultured neurons. Autophagy controls the quality of proteins or organelles; therefore, we checked whether it regulates FUS (R521C)-positive SGs. Interestingly, FUS(R521C)-positive SGs were colocalized to RFP-LC3-positive autophagosomes. Furthermore, FUS-positive SGs accumulated in atg5-/- MEFs (mouse embryonic fibroblasts) and in autophagy-deficient neurons. However, FUS(R521C) expression did not significantly impair autophagic flux. Moreover, autophagy activation with rapamycin reduced the accumulation of FUS-positive SGs in an autophagy-dependent manner. Rapamycin further reduced neurite fragmentation and cell death in neurons expressing mutant FUS under oxidative stress. Recently, we have generated induced pluripotent stem cells(iPSCs) from skin fibroblasts of ALS patients with FUS (H517Q) and differentiated ALS-linked iPSCs into neurons. SGs more accumulated in ALS iPSC-derived neurons upon oxidative stress compared to control iPSC-derived neurons. Furthermore, autophagy activation by rapamycin significantly reduced ALS-linked FUS positive SGs in ALS iPSC-derived neurons. Overall, we provide a novel

pathogenic mechanism of ALS associated with a FUS mutation under oxidative stress, as well as therapeutic insight regarding FUS pathology associated with excessive SGs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO2-1**
발표분야: Frontiers in Chemical Biology
발표종류: 분과기조강연, 발표일시: 금 09:00, 좌장: 정상전

Neurons on Nanotopographies

최인성

KAIST 화학과

Topography, the physical characteristics of an environment, is one of the most prominent stimuli neurons can encounter in the body. Many aspects of neurons and neuronal behavior are affected by the size, shape, and pattern of the physical features of the environment. A recent increase in the use of nanometric topographies, due to improved fabrication techniques, has resulted in new findings on neuronal behavior and development. Factors such as neuron adhesion, neurite alignment, and even the rate of neurite formation have all been highlighted through nanotopographies as complex phenomena that are driven by intricate intracellular mechanisms. The translation of physical cues is a biologically complex process thought to begin with recognition by membrane receptors as well as physical, cell-to-surface interactions, but the internal biological pathways that follow are still unclear. In this respect, nanotopography would be a more suitable platform on which to study receptor interfaces than microtopography because of the subcellular topographical features that are relevant in scale to the receptor activity. Ultimately, the characterization of this unknown network of pathways will unveil many aspects of the behavior and intracellular processes of neurons, and play an important role in the manipulation of neuronal development for applications in neural circuits, neuroregenerative medicine and prostheses, and much more.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO2-2**
발표분야: Frontiers in Chemical Biology
발표종류: 심포지엄, 발표일시: 금 09:35, 좌장: 정상전

Identification of Cellular Target for the Synthetic Analogue of Natural Product Regulating HIF-1α Expression

안종석

한국생명공학연구원 항암물질연구단

Rapid proliferation of cells in solid tumors causes various extents of hypoxia, oxygen-deprived states in the tissue. Cancer cells under hypoxia accumulate a gamut of proteins via transcriptional induction, which supports growth of tumor tissues and promotes resistance to cell death. These proteins play critical roles in controlling angiogenesis, cell proliferation, glucose uptake, apoptosis, and metastasis. The transcriptional induction of these genes is mediated by the master regulator of transcription factor, hypoxia-inducible factor (HIF)-1, which results in selection of cancer cells that are adapted to hypoxic conditions. HIF-1 is a heterodimeric protein composed of HIF-1α and HIF-1β subunits. The alpha subunit is continuously transcribed and translated, and its stability is regulated by oxygen level. The activity of HIF-1 is regulated by the stability of the alpha subunit that accumulates under hypoxia but is rapidly degraded unlike the beta subunit under normoxia. The accumulation of HIF-1α is prerequisite condition for the activity of HIF-1, which has become an important cancer therapeutic target.

Moracin O with an arylbenzofuran ring isolated from Morus species is a natural product and it exerts potent inhibitory effect on HIF-1 accumulation under a hypoxic condition. The exact molecular target or underlying mechanism of moracin remains unknown, which is bottleneck for further development of moracin as novel anticancer agent. Synthetic methodology for moracin previously developed and a novel and potent analogue obtained which potently suppressed hypoxia-induced HIF-1α accumulation in Hep3B cells. Accordingly using a synthetic derivative, we identified its molecular target and subsequently elucidated its role in HIF-1α accumulation through an affinity capture method followed by identification of putative target proteins by mass spectrometry, chemical-protein binding assay and various biological assays.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO2-3**
발표분야: Frontiers in Chemical Biology
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 정상전

A Novel Small-Molecule Inhibitor Targeting the IL-6 Receptor β Subunit, Glycoprotein 130

최용석

고려대학교 생명과학대학

IL-6 is a major causative factor of inflammatory disease. Although IL-6 and its signaling pathways are promising targets, orally available small-molecule drugs specific for IL-6 have not been developed. To discover IL-6 antagonists, we screened our in-house chemical library and identified LMT-28, a novel synthetic compound, as a candidate IL-6 blocker. The activity, mechanism of action, and direct molecular target of LMT-28 were investigated. A reporter gene assay showed that LMT-28 suppressed activation of STAT3 induced by IL-6, but not activation induced by leukemia inhibitory factor. In addition, LMT-28 downregulated IL-6-stimulated phosphorylation of STAT3, gp130, and JAK2 protein and substantially inhibited IL-6-dependent TF-1 cell proliferation. LMT-28 antagonized IL-6-induced TNF-α production in vivo. In pathologic models, oral administration of LMT-28 alleviated collagen-induced arthritis and acute pancreatitis in mice. Based on the observation of upstream IL-6 signal inhibition by LMT-28, we hypothesized IL-6, IL-6Rα, or gp130 to be putative molecular targets. We subsequently demonstrated direct interaction of LMT-28 with gp130 and specific reduction of IL-6/IL-6Rα complex binding to gp130 in the presence of LMT-28, which was measured by surface plasmon resonance analysis. Taken together, our data suggest that LMT-28 is a novel synthetic IL-6 inhibitor that functions through direct binding to gp130. Herein, our work on discovery of novel first-in-class gp130 inhibitors as potential therapeutic agents for the treatment of inflammatory diseases will be presented.

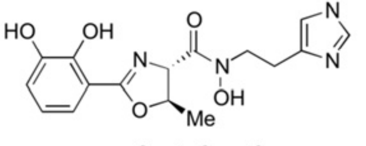
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO2-4**
발표분야: Frontiers in Chemical Biology
발표종류: 심포지엄, 발표일시: 금 10:35, 좌장: 정상전

Studies towards understanding chemistry and biology of siderophore-antibiotic conjugates

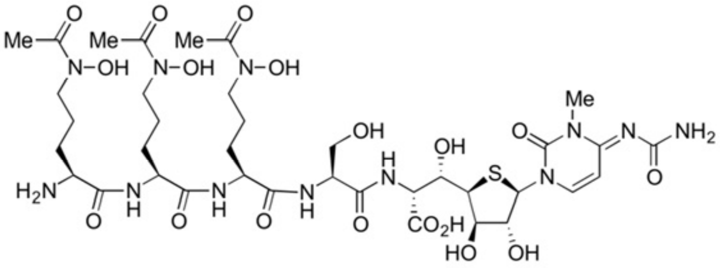
김학중* 송운영 정다와 박예송 이민욱 황진효

고려대학교 화학과

The concept of the utilization of siderophores, bacterial iron scavengers, as antibiotic delivery vehicles has been attracting significant attentions as an alternative and promising approach to overcome serious issues associated with drug-resistant bacterial infections. Although various efforts to discover potent natural and artificial siderophore-antibiotic conjugates – often called “sideromycins” – have been pursued over the decades, none has yet to reach clinics. To find some breakthroughs from this disappointing situation and also to explore the enormous potential of the sideromycin concept, we have systematically investigated chemistry and biology of some siderophore-antibiotic conjugates. Specifically, in this presentation, our current efforts to understand the capability of acinetobactin, a native siderophore of *Acinetobacter baumannii*, as an antibiotic delivery vector as well as to elucidate the biosynthetic mechanisms of a natural sideromycin, albomycin δ_2, isolated from *Streptomyces sp.* Strain ATCC 700974 will be discussed.



acinetobactin



albomycin δ_2

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN1-1**
발표분야: Current Trends in Organic Chemistry I: Methodology and Application
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 이희승

Copper(I)-Catalyzed Methods for the Synthesis of Organoboron Compounds: Development and Asymmetric Catalysis

윤재숙

성균관대학교 화학과

Organoboron compounds are useful intermediates in organic chemistry and increasing efforts have been made to establish their efficient synthesis. Transition-metal catalyzed additions of boron reagents to carbon–carbon multiple bonds have become important tools for the synthesis of organoboron compounds. Especially, enantioselective copper-catalyzed addition of boron reagents has been extensively investigated.

This presentation will describe our recent development of copper-catalyzed methods for the stereoselective synthesis of organoboron compounds. Strategies towards developing asymmetric catalyses using chelating phosphine–copper catalysts and scope of the methods will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN1-2**

발표분야: Current Trends in Organic Chemistry I: Methodology and Application

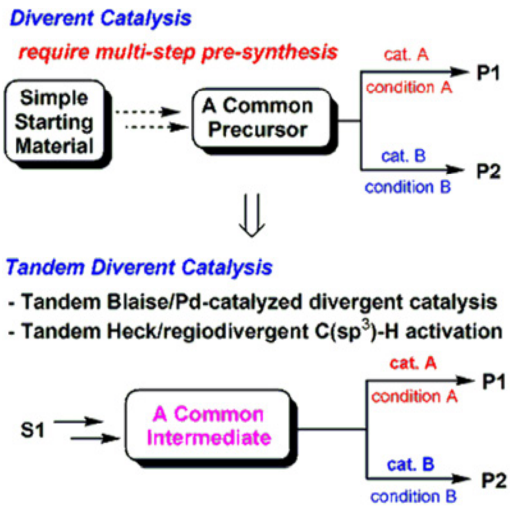
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이철범

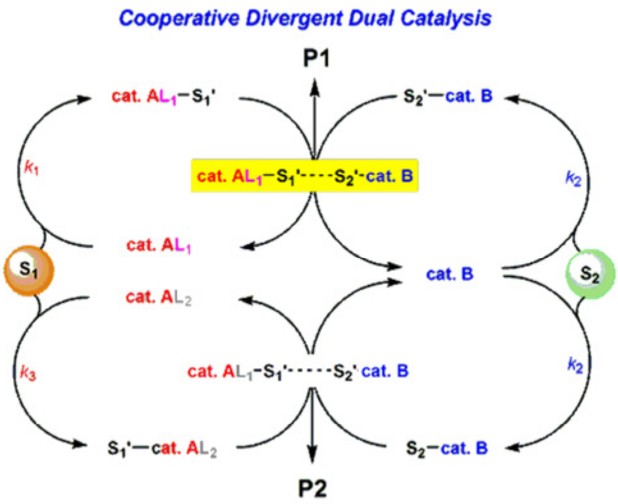
Divergent Catalysis

이상기

이화여자대학교 화학/나노과학과

Divergent catalytic reactions provide quick access to structurally diversified compounds from a common precursor, and are highly attractive tools in the discovery of drugs and functional materials.[1] A more promising yet challenging strategy that remains largely unexplored is tandem divergent catalysis, which combined the key advantages inherent to both tandem reaction and divergent catalysis to provide a rapid access to diversified structures from the same simple reagents while minimizing generation of waste. In this symposium, two different types of tandem divergent catalysis will be presented, i.e., (i) Tandem Blaise/Pd-catalyzed divergent catalysis.[2] (ii) Tandem Heck/Pd-solvent controlled regiodivergent C(sp3)-H bond activation. Our recent discovery of cooperative Pd(0)/Rh(II) dual catalysis that made possible to achieve divergent [3+3] and [4+3] cycloaddition reactions between π-allyl Pd(II)-complex and α-imino Rh(II)-carbenoid affording oxazines and oxazepines will also be presented. References[1]. Review: Duma, A. M.; Bode, J. W. Angew. Chem. Int. Ed. 2012, 51, 10954.[2]. (a) Review: Kim, J. H.; Ko, Y. O.; Bouffard, J. Lee, S.-g. Chem. Soc. Rev. 2015, 44, 2489. (b) Kim, J. H.; Bouffard, J. Lee, S.-g. Angew. Chem. Int. Ed. 2014, 53, 6435. (c) Kim, J. H.; Choi, S. Y.; Bouffard, J.; Lee, S.-g. J. Org. Chem. 2014, 79, 9253.


Diverent Catalysis
require multi-step pre-synthesis
Simple Starting Material
A Common Precursor
cat. A
condition A
P1
cat. B
condition B
P2
⇓
Tandem Diverent Catalysis
- Tandem Blaise/Pd-catalyzed divergent catalysis
- Tandem Heck/regiodivergent C(sp3)-H activation
S1
A Common Intermediate
cat. A
condition A
P1
cat. B
condition B
P2


Cooperative Divergent Dual Catalysis
P1
cat. AL1–S1'
S2'–cat. B
k1
cat. AL1–S1'----S2'-cat. B
k2
cat. AL1
S1
cat. B
S2
cat. AL2
k3
cat. AL1-S1'-----S2' cat. B
k2
S1'–cat. AL2
S2–cat. B
P2

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN1-3**
발표분야: Current Trends in Organic Chemistry I: Methodology and Application
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 이철범

Small-Molecule Ammonium Compounds as Enantioselective Catalysts and a Platform for Mechanitic Investigations

Amir H. Hoveyda

Boston College, Merkert Chemistry Center, Chestnut Hill, Massacussetts, 02467, USA

In this Lecture, small organic molecules that catalyze reactions of unsaturated organoboron reagents with imines and carbonyls will be introduced; products are amines and alcohols of high enantiomeric purity, intermediates used to synthesize many biologically active molecules. A distinguishing feature of the catalyst class is a proton embedded within their structure; the resulting electronic activation and structural organization play a key role in every stage of the carbon-carbon bond forming processes; this includes achieving high rates of catalyst regeneration and product release, typically obtained through rapid ligand exchange with metal-containing systems. The catalyst is derived from the abundant amino acid valine and may be prepared in large quantities in four steps with cheap chemicals. Reactions are scalable and do not demand stringent conditions and are complete within a few hours, furnishing products typically in >85% yield and ≥97:3 enantiomeric ratio (er). Moreover, it will be demonstrated that this catalyst class has been utilized for examination of key mechanistic principles that serve as the foundation for the development of versatile new methods. Among these is the use of catalyst-controlled 1,3-borotropic shifts in the development of diastereo- and enantioselective crotyl additions to imines and evaluation of various electrostatic interactions involving organofluorine compounds resulting in exceptionally efficient and selective allyl additions to fluoroketones.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN1-4**
발표분야: Current Trends in Organic Chemistry I: Methodology and Application
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 이철범

Advancing Innovation in Pharmaceutical Process Chemistry—The Synthesis of MK-3682

Ji Qi

Process Research & Development, Merck Sharp & Dohme

Developing synthetic processes for the large scale production of pharmaceuticals is becoming more challenging, with increasing pressures for lower cost and more environmental friendly methods. Our mission is to discover, develop and provide innovative and practical chemical syntheses that enables sustainable access of medicines to the world's population. This presentation describes our approach to the development of a long-term manufacturing route to an HCV NS5b inhibitor (MK-3682).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN2-1**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 윤주영

Highly branched carbohydrate-bearing amphiphiles for membrane protein research

채필석

한양대학교 생명나노공학과

Detergents are amphipathic chemicals essential for membrane protein study. Conventional detergents are widely used, but many membrane proteins surrounded by these agents tend to undergo denaturation/aggregation, leading to structural degradation and functional loss. Recently, based on detergent design principles established in our group, we have developed several classes of novel amphiphiles to overcome the limitations of conventional detergents. Among these agents, we introduce here penta-saccharide-bearing amphiphiles (PSA/Es) bearing the new hydrophilic group where a glucose core is radially surrounded by four glucose units. These agents were remarkably capable of retaining the native structures of multiple membrane proteins including a G protein-coupled receptor (GRCR) as compared to DDM. Some representatives were also effective at stabilizing beta2AR-G protein complexes, enabling us to visualize the individual subunits of the complexes via single-particle electron microscopy. Therefore, these agents will find wide utility in membrane protein research.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN2-2**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 윤주영

Proteomimetics: Inhibitors of Protein-Protein Interactions and Beyond

Andrew J. Wilson

School of Chemistry, University of Leeds & Structural Molecular Biology, University of Leeds, UK

Nature uses a stunning selection of molecular architectures to carry out complex tasks including catalysis and cell signalling. The capability of these biopolymers derives from their ability to self-organise and present functional motifs (e.g. an active site or binding surface) through precise 3-D orientation of primary structure. Foldamers are oligomers that adopt well-defined conformations and replicate some of these features using natural and non-natural building blocks.1 Foldamers derived from aromatic oligoamides are attractive because they exhibit predictable folding patterns.2 Proteomimetics utilize suitably functionalized non-peptidic foldamers to topographically mimic the spatial orientation of the key recognition residues on an α-helix and have been used to inhibit α-helix mediated protein-protein interactions.3 Such studies represent the foundations of a framework for the elaboration of mixed proteinogenic-foldamer structures and ultimately the de novo design of complex and functional abiotic tertiary structures. This presentation will highlight our efforts to develop constrained peptides as inhibitors of α-helix-mediated PPIs4 and the implications the resultant biophysical and structural analyses have for small-molecule ligand design. It will then move onto outline research efforts to develop proteomimetic chemical probes5 and our first steps6 towards realizing a vision of more elaborate functional structures.

References
1. S. H. Gellman, Acc. Chem. Res. 1998, 31, 178-190.
2. I. Huc, Eur. J. Org. Chem. 2004, 17-29.
3.V Azzarito, K. Long, N. S. Murphy and A. J. Wilson, Nature Chem., 2013, 5, 161-173.
4.J. A. Miles, D. J. Yeo, Philip Rowell, S. Rodriguez-Marin, C. M. Pask, S. L. Warriner, T. A. Edwards, A. J. Wilson, Chem. Sci., 2016, 7, 3694-3702.

5.A. Barnard, K. Long, H. L. Martin, J. A. Miles, T. A. Edwards, D. C. Tomlinson, A. Macdonald, A. J. Wilson, Angew. Chem. Int. Ed. , 2015, 54, 2960-2965.

6. G. M. Burslem, H. F. Kyle, A. L. Breeze, T. A. Edwards, A. S. Nelson, S. L. Warriner, A. J. Wilson, Chem. Commun., 2016, 52, 5421-5424.

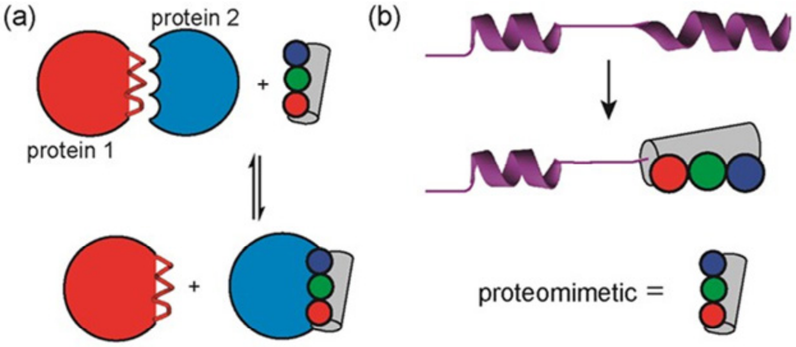


Figure 1. Functionally useful proteomimetic foldamers (a) as inhibitors of protein-protein interactions (b) towards incorporation into functional tertiary architectures.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN2-3**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 09:55, 좌장: 윤주영

Boronic Acids: Recognition, Sensing and Assembly

Tony D. James

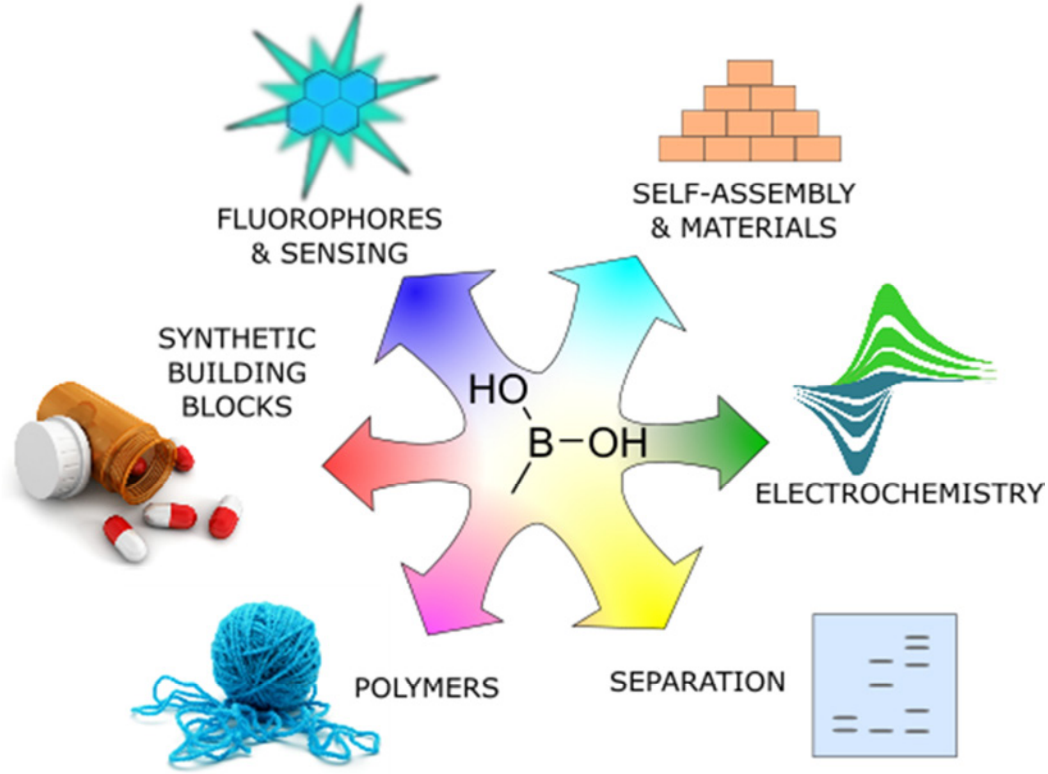
Department of Chemistry, University of Bath, UK

The ability to monitor analytes within physiological, environmental and industrial scenarios is of prime importance. Since recognition events occur on a molecular level, gathering and processing the information poses a fundamental challenge. Therefore robust chemical molecular sensors “chemosensors” with the capacity to detect chosen molecules selectively and signal this presence continue to attract considerable attention. Real-time monitoring of saccharides is of particular interest, such as D-glucose in blood. Towards that end the covalent coupling interaction between boronic acids and saccharides has been exploited with some success to monitor the presence of such saccharides. The boronic acid Lewis acid-base interaction is also suitable for the capture and recognition of anions. Anions are involved in fundamental processes in all living things. Our aim is to mimic nature’s level of sophistication in designing and producing chemosensors capable of determining the concentration of a target species such as: saccharides, glycated proteins, anions and reactive oxygen/nitrogen species (ROS/RNS) in any medium.

As well as sensors for saccharides, anions and ROS/RNS the presentation will cover the use of boronic acid based receptors for the analysis of protein glycation. Protein glycation is an important biomarker for age-related disorders such as diabetes and Alzheimer’s disease. This process whereby reducing saccharides react with amino groups of proteins ultimately leads to the formation of complex and stable advanced glycation endproducts (AGEs). Glycation compromises proteins throughout the body resulting in many diabetes related complications (e.g., nerve damage, heart attack, and blindness). Glycated proteins and their resulting AGE products are also key elements in the pathology of Alzheimer’s Disease (AD).

References

1.S. D. Bull, M. G. Davidson, J. M. H. van den Elsen, J. S. Fossey, Y. Kubo, F. Marken, A. T. A. Jenkins, Y.-B. Jiang, K. Sakurai, J. Zhao, T. D. James, Acc. Chem. Res., 2013, 46. 312–326.
2.X. Wu, Z. Li, X.-X. Chen, J. S. Fossey, T. D. James, Y.-B. Jiang, Chem. Soc. Rev, 2013, 42, 8032-8048.
3.M. Li, W. Zhu, F. Marken, T. D. James, Chem. Commun. 2015, 51, 14562-14573.
4.X. Sun and T. D. James, Chem. Rev. 2015, 115, 8001-8037.
5.X. Sun, W. Zhai, J. S. Fossey and T. D. James, Chem. Commun. 2016, 52, 3456-3469.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN2-4**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 윤주영

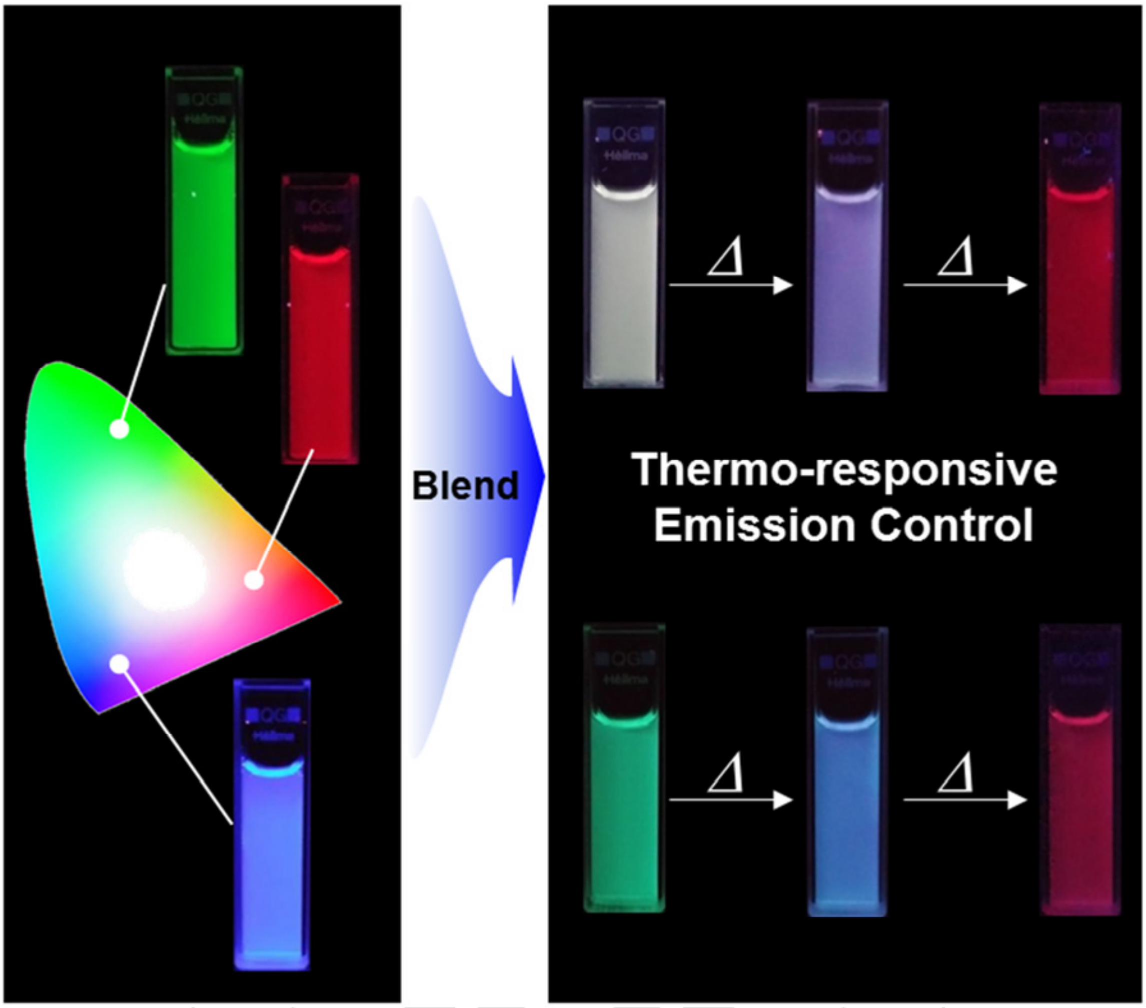
Multi-modal stimuli-responsive functional materials

장우동

연세대학교 화학과

Poly(2-isopropyl-2-oxazoline) (POx) is well known thermoresponsive polymer, which exhibits a reversible and rapid hydrophilic-hydrophobic interconversions through the lower critical solution temperature (LCST). Narrow molecular weight distributions of POx can be achieved by cationic living polymerization of oxazoline monomer. More importantly, we can readily introduce various end functional groups to the imitation or termination ends owing to the living polymerization process. We can utilize functional initiators to introduce specific functional groups at initiation end. Alternatively, termination end can be easily modified by treating with functional nucleophile to the living cationic terminal.

Recently, we have designed multimodal stimuli-responsive dendritic-linear block copolymers and light sensitive telechelic polymers have been designed through the end functional modification of POxs. LCST of the dendritic-linear block copolymers was greatly dependent of the solution pH. Azobenzene-bearing telechelic POx exhibited multimodal stimuli responsiveness. POxs were conjugated with three representative blue, green, and red fluorescence dyes for the temperature-dependent control of fluorescence emission. The three POx-dye hybrids exhibited clear hydrophilic–hydrophobic transitions via heating and cooling processes, accompanied by emission changes. By blending of the POx-dye hybrids, fully reversible emission color controls from blue to green, green to red, and blue to red have been achieved. Furthermore, the emission color can be tuned by changing the mixing ratio of each POx-dye hybrids. These unique fluorescence-tunable systems have great potential for applications in various photonic devices and sensors. In this symposium, we are going to report details of our recent research on multimodal stimuli responsive POxs.


Blend
Thermo-responsive
Emission Control
Δ
Δ
Δ
Δ

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN3-1**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 홍순혁

Development of New Methodologies for Aromatics and Heteroaromatics

이용록

영남대학교 화학공학부

Aromatics and heteroaromatics are of great importance for pharmaceuticals, agrochemicals, dyes, and advanced materials. Owing to their importance and usefulness, a number of methods for the synthesis of aromatics and heteroaromatics have been reported. Among these, transition-metal-catalyzed annulation reactions are now well-established, but the majority suffers from certain drawbacks including the necessity of complex and expensive metal catalysts and harsh reaction conditions. Therefore, more environmentally benign, cheaper, and milder alternatives are highly desirable to improve on these shortcomings. Herein, I present unique development for the construction of various functionalized and diverse aromatics and heteroaromatics such as biaryls, terphenyls, 2-hydroxybenzophenones, pyridines, 2-pyridones, chromenopyridines, azopyrazoles, carbazoles, and indoles. These protocols offer several significant advantages, such as catalyst-free, low toxicity, ease of handling, excellent functional group tolerance, environmental benignity, and mild reaction conditions. References[1] Cai, H.; Xia, L.; Lee, Y. R. Chem. Commun. 2016, 52, 7661.[2] Paul, S.; Lee, Y. R. Green Chem. 2016, 18, 1488. [3] Poudel, T. N.; Lee, Y. R. Chem. Sci. 2015, 6, 7028. [4] Poudel, T. N.; Lee, Y. R. Org. Lett. 2015, 17, 2050.[5] Poudel, T. N.; Lee, Y. R.; Kim. S. H. Green Chem. 2015, 17, 4579.

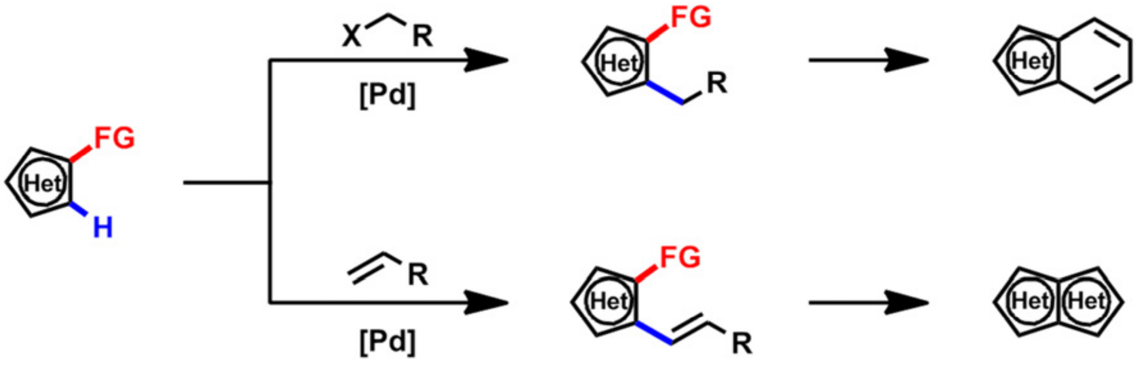
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN3-2**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 14:05, 좌장: 홍순혁

Pd-catalyzed C−H Functionalization Reactions for the Synthesis of Complex Heteroarenes

주정민

부산대학교 화학과

Heteroarenes are a ubiquitous structural motif of new pharmaceuticals, agrochemicals, and functional materials. Thus, the development of methods for the synthesis of structurally diverse heteroarenes represents an important objective in organic synthesis. We have developed Pd-catalyzed C–H functionalization reactions of substituted heteroarenes. The modification of the electronic nature of the heterocyclic ring with electron-withdrawing groups facilitated C–H alkylation and alkenylation of pyrazoles and indoles. Readily available allyl acetates, benzyl chlorides, α-haloacetates, and alkenes were employed as alkyl and alkenyl group donors in these C–C bond forming reactions to provide multi-substituted heteroarenes. Furthermore, the resulting products underwent cyclization reactions to afford fused heteroarene rings. This strategy based on C–H functionalization complements other cyclization methods and allows the systematic preparation of new, highly functionalized heterocyclic compounds.



C–C Bond Formation of Functionalized Heteroarenes

New Strategy for the Synthesis of Fused Heteroarenes

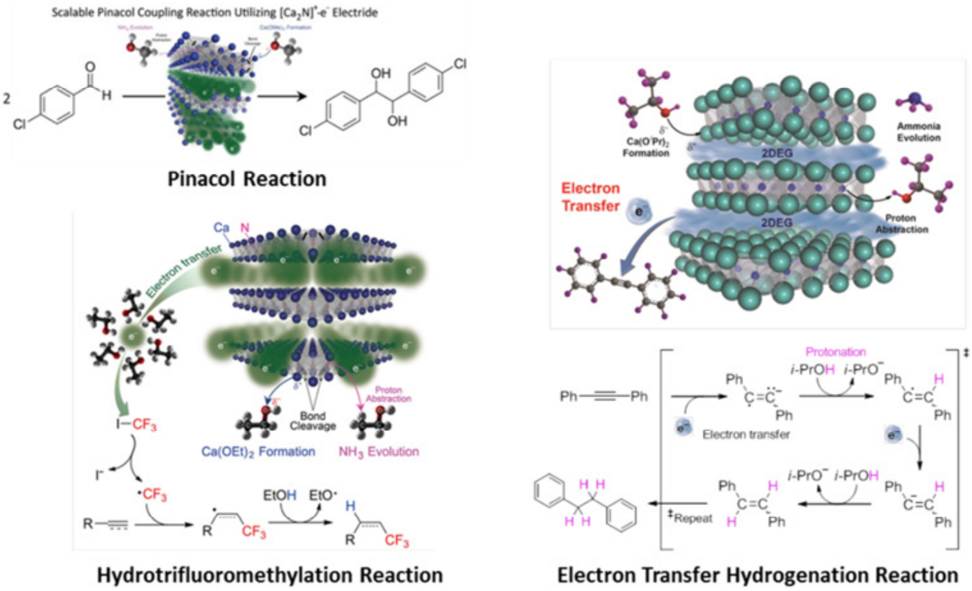
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN3-3**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 14:40, 좌장: 홍순혁

Inorganic Electride as Tool for Pinacol Coupling, Transfer Hydrogenation and Hydrotrifluoromethylation Reactions

양정운

성균관대학교 에너지과학과

Two-dimensional electride $[Ca_2N]^+$•e–, which has anionic electron layers between cationic framework layers ($[Ca_2N]^+$), has recently emerged as an effective electron donor in synthetic organic chemistry. It has small work function (2.6 eV) and high electron concentration ($\sim 1.37 \times 10^{22}$ cm^{-3}) similar to those of typical alkali metals. We recently demonstated the pinacol coupling reaction of aldehyde, the electron transfer hydrogenation of alkyne and alkene, and the hydrotrifluoromethylation reaction of alkene and alkyne with trifluoromethyl iodide utilizing the two-dimensional electride $[Ca_2N]^+$•e– as an electron donor (Scheme 1). The detailed reaction mechanisms will be provided in the presentation.



Pinacol Reaction

Hydrotrifluoromethylation Reaction

Electron Transfer Hydrogenation Reaction

Scheme 1. Pinacol coupling reaction, transfer hydrogenation reaction, and hydrotrifluoromethylation reaction utilizing two-dimensional electride $[Ca_2N]^+ \cdot e^-$ as an electron donor

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MEDI-1**

발표분야: Innovative Trials and Technology for Drug Discovery

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이태호

Identification and chracterization of novel small molecule suppressor and inducer of intracellular reactive oxygen species as a potential neuroprotective agent and a potential anticancer agent

허우영

한국과학기술연구원(KIST) 화학 키노믹스 연구센터

Oxidative stress induces cell death. As a consequence, chronic exposure of oxidative stress causes tissue damage and ultimately leads to diseases including neurological disorders. But because of the fact that cancer cells are more sensitive to oxidative stress relative to normal cells, induction of oxidative stress can be a good strategy for selective cancer eradication. Here I would like to introduce a novel class of Nrf2 activator (namely AI-1) identified from cellular screening of small molecule library, which serves as an antioxidant and protects cells from reactive oxygen species (ROS), and a natural ROS inducer (irisquinone), which shows a selective cytotoxicity to cancer cells. AI-1 irreversibly modifies Cys151 of Keap1 and disrupts the ability of Keap1 to serve as an adaptor for Cul3-Keap1 ubiquitin ligase complex, thereby causing stabilization and transcriptional activation of Nrf2. Irisquinone is a 17-carbon chain-tethered quinone species, and interestingly our biochemical study indicated that 17-carbon chain is crucial for ROS production and a selective, potent anticancer effect.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MEDI-2**

발표분야: Innovative Trials and Technology for Drug Discovery

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이태호

Design and Synthesis of selective multi-kinase inhibitors for EGFR and angiokinases

민경훈

중앙대학교 약학대학

Antiangiogenic agents have been investigated in combination with standard chemotherapy or targeted cancer agents for better management of advanced cancers. Therapeutic agents that inhibit EGFR and other angiokinases could be useful alternatives to combination therapies for EGFR dependent cancers. Herein, the synthesis of indole derivatives of pazopanib using a bioisosteric replacement strategy are described, which was designated MKP101 as a selective multi-kinase inhibitor. A docking model of MKP101 and the kinase domain of the EGFR was generated to predict its binding mode, and validated by synthesizing and evaluating MKP101 derivatives. Moreover, a study of structure-activity relationships of indolylamino or indolyloxy pyrimidine analogues derived from MKP101 demonstrated that selectivity for EGFR and other angiokinases, especially VEGFR-2 depends on the position of substituents on pyrimidine and the type of link between pyrimidine and the indole moiety. This study could provide a basis for developing angiokinases inhibitors having high affinity for EGFR, from the pyrimidine scaffold.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI-3**
발표분야: Innovative Trials and Technology for Drug Discovery
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 민경훈

AptaBio Therapeutics Inc.; Platform Technology, drug discovery and development Pipelines

문성환

Aptabio Therapeutics CTO

AptaBio Therapeutics Inc. is a research based pharmaceutical company that discovers and develops innovative medicines.AptaBio has extensive experience in the drug discovery research developing selective inhibitors of the NADPH oxidase (NOX) enzymes and aptamer based anti-cancer drug. This position has been built upon the development of a specialist and proprietary assay platform which supports the screening and design of novel molecules against new targets. •AptaBio's focused targets are the potential use of NADPH oxidase inhibitors to treat diabetic complications and aptamer drug conjugates to treat cancer. •AptaBio has a unique and proprietary screening platform and pipeline with a first in class drug candidate, APX-115 to treat diabetic nephropathy (DN). In parallel, AptaBio is using its Nox platform to develop new inhibitor, APX-5278 with different Nox selectivity which can address Atherosclerosis. •AptaBio is using its Nox platform to develop new inhibitor, APX-1004 which can address diabetic retinopathy. And, AptaBio is using its Nox platform to develop new inhibitor, APX-311 which can address NASH. •Aptabio is using aptamer drug conjugate to develop anti-cancer drug, Apta-12 which can address solid tumor like as pancreatic cancer and Apta-16 which can address blood tumor like as AML . This symposium will provide an overview of AptaBio Therapeutics Inc.'s platform technology, drug discovery and development pipelines and discuss the latest advances.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI-4**
발표분야: Innovative Trials and Technology for Drug Discovery
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 민경훈

Controlling Specificity of Receptor Tyrosine Kinase Signaling

배재현

대구경북첨단의료산업진흥재단 신약개발지원센터

Kinases play crucial roles in many fundamental biological processes like cell proliferation, embryonic development, and cell death. Therefore, aberrant functions of kinases cause severe consequences including malignancies, and developmental disorders. Their biological roles in cell signaling are controlled by selective recruitment and phosphorylation of specific downstream substrates.In enzymatic reaction, kinases transfer• gamma-phosphate of ATP to hydroxyl group of Ser/Thr or Tyr residue according to their substrate preferences. Ser/Thr kinases recognize their substrates through negatively charged regions positioned in vicinity of substrate binding site interacting to the positively charged residues (Arg, Lys) near the substrate Ser/Thr. In contrast, Tyr kinases selectively recruit their substrate through positively charged regions of Tyr kinases interacting with negatively charged residues (Glu, Asp) near the substrate Tyr.In this study, the preliminary result shows that Ser/Thr kinase phosphorylates Tyr by switching the negatively charged regions of S/T kinase near the substrate binding site to positively charged residues. This preliminary result supports that Ser/Thr and Tyr kinases utilize opposite charge distribution on their catalytic clefts as one of their “proof reading” procedures to select the right substrates.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT1-1**
발표분야: Nanobio-materials for Biomedical Application
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 박종남

Cell Signalling Control by using Magnetic Nanoparticles

유동원

연세대학교 화학과

Controlling of cellular activities in a space and time selective manner is one of the challenging issues in biomedical science. In contrast to biochemical ligands, magnetic nanoparticles have the potential of cellular activity modulation with spatio-temporal controllability. When magnetic nanoparticles are exposed to external magnetic field, these particles can generate mechanical forces (*e.g.*, gradient force and inter-particle force) or heat. These kinds of energies can be used to initiate cell signaling in biological systems, which can manipulate cellular activities (*e.g.*, cell death). In this talk, I'll present that magnetic nanoparticles can control cell fate in a remote and precise fashion.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT1-2**

발표분야: Nanobio-materials for Biomedical Application

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 박종남

Multi-Functional Hydrogels for Biomedical Applications

차채녕

울산과학기술원 신소재공학부

Hydrogels are widely used in biomedical applications, such as biosensing, drug delivery, pharmaceutics, and tissue engineering. In order to account for the complexities of biological systems, these materials must be adaptable to specific purposes with efficiency, precision, and versatility. Therefore, the focus of my research has been geared towards engineering multi-functional hydrogels by synthesizing novel biopolymers and utilizing microfabrication techniques. In this presentation, several topics related to hydrogel microfabrication will be covered, including (1) oxidized methacrylic alginate (OMA) to develop hydrogels whose mechanical, diffusional, and degradation rate can be controlled independently, (2) polyaspartamide-based linkers that conjugate bio-functional moieties (e.g. peptides, proteins) in a single step to a material of choice for specific biological responses, (3) fabrication of core-shell microgels using a microfluidic device, and (4) fabrication of three dimensional tissue constructs using a Digital Micromirror Device (DMD)-based 3D printing technique.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT1-3**

발표분야: Nanobio-materials for Biomedical Application

발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 박종남

Nano-biomaterials for stem cell differentiation and cellular reprogramming

조승우

연세대학교 생명공학과

Stem cells have shown huge potential as therapeutics for the treatment of incurable diseases, but their therapeutic efficacy needs to be further improved by enhancing specific lineage differentiation required for tissue regeneration. Direct reprogramming can also contribute to generation of tissue-specific cell types for therapeutic applications, but low efficiency of conversion still remains a major challenge. In this presentation, different types of nano-biomaterials will be introduced to promote neuronal differentiation of stem cells and direct conversion of fibroblast to neuronal lineage cells. Microfluidic devices and nanoscale pattered substrates for the reconstitution of neural stem cell microenvironments are reported to promote functional neuronal differentiation of human neural stem cells. In addition, micro-devices generating external stimulation and allowing for microenvironmental control are used for enhancing the efficiency of polymer nanoparticle-mediated direct conversion of fibroblasts to functional induced neuronal cells and reducing the time scale required for the conversion process. The nano-biomaterials reported herein can provide biomedical platforms for improving stem cell therapy and reprogramming strategies for the treatment of neurodegenerative diseases.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT1-4**
발표분야: Nanobio-materials for Biomedical Application
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 유자형

Versatile underwater adhesive with microarchitecture triggered by solvent exchange

이동욱

UNIST 에너지 및 화학공학부

Polyelectrolyte complexation is critical to the formation and properties of many biological and polymeric materials, and is typically initiated by aqueous solution mixing that results in fluid-fluid phase separation, e.g., coacervation. Here we report a versatile and strong wet-contact adhesive inspired by sandcastle worm cement that enables both a triggered complexation of polyelectrolytes, and formation of a porous architecture. A catechol-functionalized weak poly-anion was premixed with a poly-cation in dimethyl sulfoxide (DMSO). The polymer solution was applied underwater to substrates where electrostatic complexation, phase inversion, and rapid setting were actuated by water-DMSO solvent exchange. This process offers enhanced spatial and temporal control of complexation, thereby fostering rapid (≥ 25 s) and robust underwater adhesion of complexed catecholic polyelectrolytes to all tested surfaces including plastics, glasses, metals, and biological surfaces. The solvent exchange process is adaptable to diverse materials chemistry, supporting functionalities well beyond aqueous complex coacervates.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT1-5**

발표분야: Nanobio-materials for Biomedical Application

발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 유자형

Liporaxel® (DHP107), the first-generation oral paclitaxel delivery system

이인현

대화제약 판교연구소

The first successful oral paclitaxel formulation, Liporaxel® (DAEHWA Pharm. Co., DHP107), has been prepared by dissolving paclitaxel in the mixture of non-toxic lipid excipients and surfactants using DH-LASED® (**D**ae **H**wa **L**ipid b**A**sed **S**elf **E**mulsifying **D**rug delivery) technology. Unlike the conventional oral paclitaxel dosage forms under development, DHP107 was effectively absorbed in the intestinal tract without concurrent use of P-glycoprotein inhibitors such as cyclosporine A, SDZ PSC 833, and HM30171A. In a rodent xenograft preclinical cancer model, the bioavailability of Liporaxel® (DHP107) was about 50 % as compared to I.V. paclitaxel. Moreover, the preclinical trials of Liporaxel® (DHP107) showed excellent antitumor efficacy and demonstrated its safety in toxicology study. Subsequently, we successfully completed its clinical studies up to phase 3. The clinical studies of Liporaxel® (DHP107) re-confirmed its efficacy and safety in gastric cancer patients as compared to the I.V. paclitaxel. Overall, we believe that the Liporaxel® (DHP107) is able to improve therapeutic efficacy of the P.O. paclitaxel administration and further the quality of life of cancer patients and family.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT1-6**

발표분야: Nanobio-materials for Biomedical Application

발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 유자형

Bioinspired Synthetic Inorganic Nanoparticles for Bone Tissue Engineering

HWANG NATHANIEL SUKYEON

서울대학교 화학생물공학부

Recently, synthetic matrices emulating the physiochemical properties of bone tissues are being developed to control stem cell fate. Biomaterials containing calcium phosphate moieties, such as hydroxyapatite (HAP: $Ca_{10}(PO_4)_6(OH)_2$), have been shown to induce osteogenic differentiation of stem/progenitor cells and bone tissue formation. Recent evidences suggest that one of the main components of inorganic phase of bone is whitlockite (WH: $Ca_{18}Mg_2(HPO_4)_2(PO_4)_{12}$). Even though WH a relatively rare mineral in nature, it is the second most abundant mineral in human bone with approximately upto 20 wt%, and it is particular found in bone with elevated dynamic loading. The increased detection of short micro-ranged WH in bone under increased loading along with its acidic stability suggests that it may act as an inorganic template composition for further mineralization. In addition, elevated composition of WH in adolescent's bone suggest that it may be actively involved in bone remodeling process. Here, we investigated the role of WH on bone formation. WH nanoparticles were synthesized, and we demonstrate that the synthetic WH can recapitulate early-stage bone regeneration via elevated extracellular PO_4^{3-} and Mg^{2+} concentration. Furthermore, our studies showed that WH participates in bone formation via increased affinity with extracellular proteins. Finally, we demonstrated that the WH containing scaffold platform could stimulate in vivo bone formation. The multidisciplinary approach conducted in this study provided an organized methodology to find biological functionalities of WH and introduced a useful clinical application of WH for bone formation.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

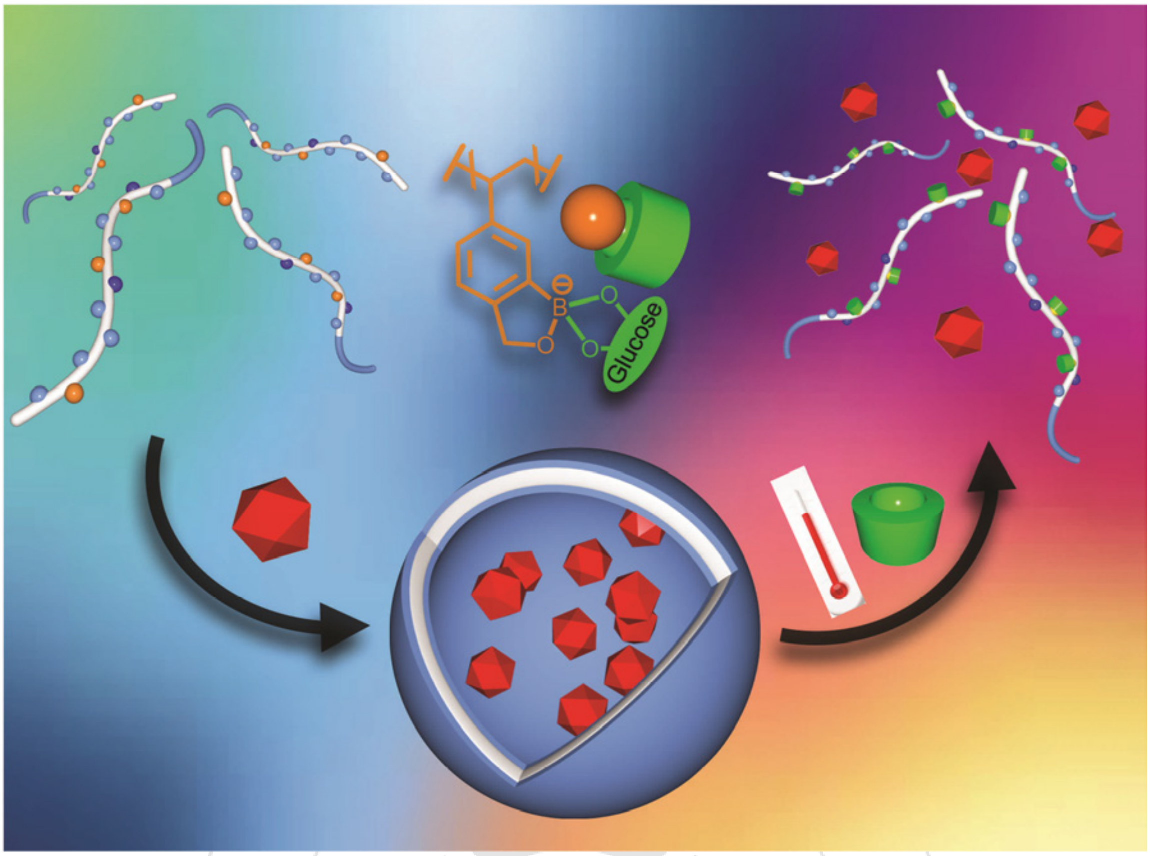
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT2-1**
발표분야: Responsive Smart Materials
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 박소정

Monosaccharide-Responisive Polymers and Polymer Nanostructures

김경택

서울대학교 화학부

Organobobonic acid-containing polymers and block copolymers have recently attracted attention because of their ability to recognize important natural diol compounds such as saccharides and nucleotides under physiologically relevant conditions at neutral pH. In particular, polymers and block copolymers that are responsive toward multiple stimuli can be utilized to create smart delivery vehicles for use in applications in a complex environment. We have studied polymers containing boronic acid and its derivatives that are responsive toward biologically important diols. Utilizing controlled radical polymerization techniques, well-defined block copolymers containing benzoboroxole have been synthesized, and their self-assembly in water have also been studied. Here we report that self-assembled nanostructures of boroxole-containing block copolymers could serve as delivery vehicles and nanomaterials that respond to the presence of biologically important diols such as glucose and ATP. Synthesis of block copolymers showing responsiveness toward multiple stimuli will also be discussed.


B
O
O
O
O
Glucose

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT2-2**

발표분야: Responsive Smart Materials

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 박소정

Chameleon-Inspired Mechanochromic Photonic Skins Composed of Colloidal Crystals

김신현

KAIST 생명화학공학과

Chameleons exhibit rapid color change during social communications. This remarkable talent is contributed from a lattice of guanine nanocrystals in their skin. The lattice reflects selected wavelength of light depending on the lattice constant and chameleons control the structural color by modulating the lattice constant. Inspired from chameleons, we have designed photonic films composed of nonclose-packed colloidal crystals embedded in an elastic polymer matrix. To produce the colloidal crystals, monodisperse silica particles are dispersed in a photocurable resin that causes interparticle repulsion by disjoining pressure. The silica particles spontaneously assemble into the nonclose-packed face-centered cubic (fcc) structure to minimize total repulsive energy, which is then captured in a polymer matrix by photocuring the resin. The resulting film displays structural colors as the fcc lattice possesses a photonic bandgap property. More importantly, the color can be dynamically and reversibly tuned by elastic deformation of the film. As the film is laterally stretched up to yield strain, the color is blue-shifted in entire visible range. For vertical compression with stamps, multicolor patterns are developed from single-colored film. The elastic photonic films that resemble the chameleon skins are appealing for reflection mode display and colorimetric sensors.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT2-3**
발표분야: Responsive Smart Materials
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 박소정

Controlling Wave Transport in Periodic and Quasiperiodic Structures

허가현

한국과학기술연구원(KIST) 계산과학연구센터

Controlling the wave transport properties of materials provides opportunities for engineering better materials for a variety of applications including photonics, thermoelectrics, acoustics, and electronics. In particular, translational symmetry of materials strongly governs transport properties of every form of waves such as electron, photon, and phonon since the waves having a wavelength commensurate with crystal's periodicity can transmit without losses. In this talk, I will discuss photonic and phononic properties of periodically structured nanomaterials derived from bottom-up type block copolymer self-assembly. Peculiar wave transport behaviors of quasiperiodic structures, ordered and well-defined structures without any translation order, will be further discussed.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT2-4**
발표분야: Responsive Smart Materials
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 박소정

Metal-Inorganic Nanowires for Advanced Optical Elements

현가담

이화여자대학교 화학 나노과학과

The miniaturization of optical components to the nanoscale has been an active field of research as the integration of optics with nanoelectronics has become increasingly needed. One component of critical importance in this effort is the optical filter. Traditionally organic dyes have been used as micron-sized filters for display pixels, but these materials suffer from lifetime and stability issues. Metal grating structures relying on surface plasmon polaritons have also been demonstrated showing that a large number of gratings elements can create optical passbands where the wavelength is tunable through the period. One drawback in this scheme is that in order to achieve high transmission efficiency and reliable spectral purity a large number of grating elements is necessary, which implies a large pixel or filter size. In this talk, I will present a new concept for high-efficiency optical filters that can operate even with a single element. Wavelength tunability is achieved by varying the diameter of the nanowire, while the absolute transmission can be controlled through the number of nanowires. Such results present intriguing possibilities in nanoscale communication or ultrahigh resolution color pixels.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT3-1**
발표분야: Current Trends in Nano Materials Chemistry
발표종류: 심포지엄, 발표일시: 금 13:30, 좌장: 인수일

Highly Efficient Reduced TiO$_{2\text{-X}}$ Photocatalyst via Mg Reduction in H$_2$/Ar

유종성

DGIST 에너지시스템공학과

Recently, black TiO2-x materials were achieved by creating oxygen vacancies and/or defects at the surface using different methods.1 Fascinatingly, they exhibited an extended absorption in VIS and IR instead of only UV light with a band gap decreases from 3.2 (anatase) to ~1 eV.2 However, despite the dramatic enhancement of optical absorption of black TiO2-x material, it fails to show expected visible light-assisted water splitting efficiency.1,3 This was ascribed to the high concentration of the surface defects and/or oxygen vacancies, considered as an electron donor to enhance donor density and improve the charge transportation in black TiO21,3 can also act as charge recombination centers, which eventually decreases photocatalytic activity.3 Therefore, a black TiO2 material with optimized properties would be highly desired for visible light photocatalysis.Herein, we report reduced of TiO2-x nanoparticles prepared in the presence Mg and H2/Ar for excellent photocatalytic H2 production from methanol-water system.4 On the basis of all the results, it can be realized that The outstanding activity and stability of our RT-0.5 suggest that a balanced combination of different factors like Ti3+, surface defects, oxygen vacancy, and recombination center is achieved along with optimized band gap and band position during the preparation employing magnesiothermic reduction in the presence of H2. And the controlled magnesiothermic reduction in the presence of H2 is one of the best alternative ways to produce active and stable TiO2-based photocatalyst for H2 production.REFERENCES1. X. Chen et al., Chem. Soc. Rev. 44, 1861, (2015).2. X. Chen et al., Science, 331, 746, (2011).3. Y. H. Hu, Angew. Chem. Int. Ed., 51, 12410, (2012).4. A. Sinhamahapatra et al., Energy Environ. Sci. 8, 3539, (2015).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT3-2**
발표분야: Current Trends in Nano Materials Chemistry
발표종류: 심포지엄, 발표일시: 금 13:50, 좌장: 인수일

A Well-Defined Nanostructured, Single Crystalline TiO2 Electron Transport Layer for Efficient Planar Perovskite Solar Cells

박태호

POSTECH 화학공학과

A well-defined nanostructured TiO2 electron transport layer (ETL) with outstanding properties such as excellent transmittance, single-crystalline nature, uniform film thickness, increased effective area, high transmittance, single-crystalline nature, and defect-free physical contact with a high rough substrate leads excellent electron extraction and hole blocking ability at the planar perovskite solar cell. These result in 22 % (12.5 → 15.2 %) and 44 % (8.9 → 12.8 %) increased power conversion efficiencies (PCEs) and stabilized maximum power output efficiencies, respectively, compared with the conventional spin-coated TiO2 ETL.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT3-3**

발표분야: Current Trends in Nano Materials Chemistry

발표종류: 심포지엄, 발표일시: 금 14:10, 좌장: 인수일

AN EFFECTIVE APPROACH FOR PHOTODEACTIVATION OF HARMFUL ALGAL BLOOMS WITH VARIOUS PHOTOCATALYST UNDER SOLAR LIGHT

이수완

선문대학교 환경생명화학공학과

In recent years, semiconductor photocatalysis has attracted much attention due to its potential applications to solve the environmental problems [1]. Utilization of photocatalysis in many chemical processes is of special interest as it can be applied for the removal of toxic agents in air and water using solar energy so that photocatalytic technologies are now considered as promising technologies.

Adverse environmental effects from some marine microorganisms now seriously impact our lives. Marine microbes, which are responsible for approximately half of the Earth’s primary production of nutrients, play an enormous role in global nutrient cycling. Marine microorganisms are small, and acellular or unicellular. Some phytoplanktons are bacteria, some are protists, and most are single-celled plants. Among the common kinds are cyanobacteria, silica-encased diatoms, dinoflagellates, green algae, and chalk-coated coccolithophores. The most evident effects of these kinds of red and green tides are associated with wildlife mortalities of marine and coastal species of fish, birds, marine mammals, and cause great economic loss and ecological damages. These events are continuously observed in oceans, rivers and lakes all over the world.

Recently, TiO2 and nitrogen doped TiO2 have been synthesized for different photocatalytic process. It has been reported that microorganisms such as Escherichia coli, marine algae, fungi, and virus are inactivated by using TiO2 photocatalyst. The aim of this research is to find an alternative way to deactivate green tide by employing heterogeneous photocatalysts. In our research center for eco multi-functional nanomaterials, various photocatalysts active under UV and visible light such as binary semiconductors like TiO2, Ag3PO4, and scheelite structures such as PbMoO4, perovskite-like cuboid materials by microwave hydrothermal, sonochemical methods, for the deactivation of hazardous Harmful

Algal Blooms.

Keywords: Red Tide, Green Tide, Photocatalyst, Ocean, River, Lake

References:
[1] J. Am. Chem. Soc., 127 (2005) 1344–1345.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT3-4**
발표분야: Current Trends in Nano Materials Chemistry
발표종류: 심포지엄, 발표일시: 금 14:40, 좌장: 박태호

Interfacial Synthesis of Metal-Organic Framework Structures by Microfluidics and Hollow Mold

김동표

POSTECH 화학공학과

Continuous-flow microreaction technology has exhibited intrinsic advantages of reduced chemical consumption, design for energy efficiency, and inherently safe chemistry. In here, I present various microreactors and their applications that have been achieved at our laboratory. In this work, we demonstrated a novel nanoliter droplet-based microfluidic strategies for continuous and ultrafast synthesis of nano-, micro functional materials. Previously, we reported an ultrafast, mild and continuous synthesis of various inorganic nanomaterials of zeolite (ZSM-5). This strategy is further exploited for metal-organic framework (MOF) crystals and their heterostructures. The MOF hollow spheres were prepared by interfacial synthesis method using immiscible two liquid phases for improved enzymatic activity. The biocompatible MOFs (e.g. iron fumarate MIL-88A) are of crucial interest for applications such as controlled release of drugs, imaging or enzymatic reaction and selected for protective porous shells even under unfriendly conditions. Different types of enzymes were chosen, encapsulated inside hollow MOF spheres and tested in comparison with spheres-free enzymes. Furthermore, the multi-shell MOF structures are fabricated by automated layer-by-layer synthesis method using immiscible two micro-droplet phase for tandem catalysis. In addition, various MOFs microstructures could be directly prepared by micro-interfacial synthesis methodology with hollow mold, then readily transferred the patterns on various substrates.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT3-5**
발표분야: Current Trends in Nano Materials Chemistry
발표종류: 심포지엄, 발표일시: 금 15:00, 좌장: 박태호

Solar Fuel: Converting CO_2 into Fuel and Chemicals

인수일

DGIST 에너지 시스템 공학 전공

The use of sunlight for the photoconversion of CO_2 and water-vapor into hydrocarbon fuels offers a practical means of storing solar energy and minimizing, or reducing, atmospheric CO_2 concentrations, hence is a topic of considerable scientific interest.

This talk describes various hybrid photocatalysts and their application to the photocatalytic conversion of CO_2 to hydrocarbon fuels. For example, The synthesis and design of a mesoporous noble metal free p-type Cu_2ZnSnS_4 (CZTS)/n-type TiO_2 heterojunction photocatalyst for broad spectrum light absorption enhanced charge separation and transfer that, in turn, enhances photocatalytic CO_2 conversion. Key factors contributing to the enhanced photocatalyst performance include improved solar-spectrum light absorption, high surface area, and rapid charge separation arising from the intrinsic p-n junction nature of the material.

The strategy of applying hybrid heterojunctioned photocatalysts offers, we believe, an excellent pathway for achieving improved photocatalytic materials with, following our specific interest, application to the photoconversion of CO_2 to fuel: that is, solar fuels.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ELEC1-1**

발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry I

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 김주훈

Chemical sensing with nanopores. A quantitative approach

Róbert E. Gyurcsányi[*] Gyula Jágerszki István Makra Péter Terejánszky Gergely Lautner Soma Papp

MTA-BME

The nanopores offer a rather unique transduction mechanism as species residing within a nanopore can effectively change the physical-chemical properties of the nanopore interior, which can be detected in a label-free manner.[1,2] By having a single nanopore delimiting a volume comparable to that of the targeted species, detection of single species becomes feasible. The detection mechanism is dominantly based on monitoring the electrical conductivity changes of the extremely small volume defined by a nanopore caused by individual species of comparable size that pass through or reside in the nanopore. These changes are generally detected by measuring the current induced by an external transpore potential in a setup that consists of two electrically connected electrolyte compartments separated by a membrane integrating a single nanopore or a nanopore array. Despite the wealth of information (e.g., size, charge, shape, etc.) and excellent size resolution that this technique can provide on single species, complex samples generally require the use of selective receptors either immobilized to the nanopore environment or added to the sample to generate responses that can be selectively distinguished from the background. Therefore, this talk will focus on the chemical modification of the nanopores and their application for quantitative analysis. Additionally, it will involve the theoretical treatment of various nanopore sensing methodologies that facilitates the understanding of the complexity of nanopore-based sensing, their prospects as well as their limitations.[3]

We will introduce calibration-free approaches for counting and sizing nanoparticles and viruses by “conventional” resistive pulse sensing, emerging as one of the most promising application area of nanopore sensors.[4,5] However, as the target species become smaller the nanopore diameters need also to be decreased, which requires the accurate assessment of extremely small currents and current changes (pA or fA) often at high time resolution. The need for highly reliable and cost effective fabrication of extremely small nanopores, as well as for demanding instrumentation and noise reduction, may therefore be limiting for genuine sensing applications. In this respect we will introduce novel methods to overcome these difficulties: (i) by inherent amplification, such as to enable the use of larger size nanopores for micro RNA detection and (ii) by potentiometric transduction, to enable quantitative analysis based on membrane potential measurements.[6,7] We found potentiometric readout, requiring solely a high input impedance voltmeter, a very practical electrochemical transduction approach for nanopore-based chemical sensors and we will demonstrate its utility for the measurement of small ions and polyelectrolytes. In this respect we will report on the smallest sensing surface potentiometric ion-selective nanoelectrodes ever fabricated to best of our knowledge. The sensing concept for detection of small ions is based on restricting the pore diameters to have the surface properties of the pore governing the transpore flux of ions, i.e., by synthesizing solid-state ion channels. For this purpose gold membranes modified with a mixed monolayer of three different thiol compounds to infer permselectivity, hydrophobicity and ion selectivity can be used as an unconventional ion-selective membrane to fabricate potentiometric ion-selective electrodes (ISEs).[6] Unlike conventional liquid membrane-based ion-selective micropipettes that have extremely limited life time (generally less than a day), the new type of single-nanopore based ISEs with all active components immobilised to the nanopore offer a much improved life time and even applicability in non-aqueous samples, Another advantage of the nanopore-based ISEs is the use of biological origin hydrophilic selective complexing agents.

References:
1.R. E. Gyurcsányi, Trac-Trend Anal Chem, 2008, 27, 627-639.
2.I. Makra and R. E. Gyurcsányi, Electrochem Commun, 2014, 43, 55-59.
3.L. Hofler and R. E. Gyurcsányi, Anal Chim Acta, 2012, 722, 119-126.
4.P. Terejánszky, I. Makra, P. Fürjes and R. E. Gyurcsányi, Anal. Chem., 2014, 86, 4688-4697.
5.P. Terejánszky, I. Makra, A. Lukács and R. E. Gyurcsányi, Electroanal, 2015, 27, 595-601.
6.G. Jagerszki, A. Takács, I. Bitter and R. E. Gyurcsányi, Angew Chem Int Edit, 2011, 50, 1656-1659.
7.I. Makra, G. Jagerszki, I. Bitter and R. E. Gyurcsányi, Electrochim Acta, 2012, 73, 70-77.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC1-2**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry I
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 김주훈

Nanoscale electrochemistry at graphite and graphene

김양래

광운대학교 화학과

Recently, tremendous research efforts have been made to study nanoelectrochemistry. However, most of researchers are not trying to elucidate electron transfer kinetics at nanoelectrodes but just focusing on electrochemical characterization of nanomaterials. There are several papers which show that electrochemical behavior of nanoelectrodes (

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC1-3**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry I
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 김주훈

Low-Power, Superfast Soft Actuators

박문정

POSTECH 화학과

In the present study, we describe a novel platform for the development of high performance ionic polymer actuators, which could be used to achieve an unprecedented fast response time under low voltage operating conditions. The actuators comprise cation-conducting block copolymers that exhibited a response time of tens of milliseconds and millimeter-scale displacement under 1 V in air, which has not been achieved by any actuators thus far. The important factor in its success involves the selective introduction of zwitterions into the nanoscale ionic domains of the polymer layer, which do not migrate under an electric field owing to the electro-neutrality. These zwitterions were designed to have structural resemblance to the polymer matrix and provide a polar medium with an exceptionally high dielectric constant of 76, thus facilitating ion dissociation and increased ion diffusivity. Accordingly, the ionic conductivities of the zwitterion-containing polymers increased 300-fold, while the single-ion conducting characteristics were preserved. We believe that these findings could enable the development of new soft actuators that can be used in the production of next-generation artificial muscles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC1-4**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry I
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 김주훈

Development of New Redox Couples for High-Performance Redox Flow Batteries

<u>변혜령</u>

KAIST 화학과

Electrochemical storage system (ESS) technology has been highly paid attention to power load control, and would be pivotal to store intermittent renewable energy sources. Redox flow batteries (RFBs) are one of the most attractive ESSs, which can be feasibly sizeable and need low maintenance. However, low energy density in commercial RFBs requiring massive electrolyte reservoirs should be much improved, which can be solved by development of promising redox couples with high solubility and redox potential. We previously demonstrated triiodide/iodide (I_3^-/I^-) redox couple in aqueous catholyte, delivering high storage capacity (~98% of the theoretical capacity), Coulombic efficiency (>99.5%) and cycling performance (>99.5% capacity retention for 100 cycles) when linked with Li metal as the anode (with nonaqueous electrolyte and impermeable separator). The high performance for aqueous Li–I_2 battery is contributed to a suitable redox potential of ~3.5 V vs. Li^+/Li in addition to high solubility, which offers a high energy density of ~0.33 kWh kg^{-1}. However, such a research direction to find 'natural and elemental style' of redox ions (e.g. vanadium ions, Zn-Br, I_3^-/I^- etc.) have a limited scope to develop RFB performance due to their intrinsic and fixed redox potential and solubility. Here we present a new research approach to design redox-couple molecules, which allows us to feasibly tune redox potentials in non-aqueous electrolyte. We employed $Co^{2+/3+}$ ion coordinated with various ligands as the redox molecules. The electron-withdrawing property of ligands and solvation with non-aqueous electrolyte modulate $Co^{2+/3+}$ redox potentials. We will discuss stability of Co-based redox molecules in this presentation, which would guide design of promising redox-couple molecules in the future.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC2-1**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry Ⅱ
발표종류: 심포지엄, 발표일시: 금 09:10, 좌장: 장진호

광(전기화학)촉매를 이용한 수소생산 및 전기화학 분석

[Photo(electro)catalytic Hydrogen Production and its Electrochemical Analysis]

박현서* **윤창원**

한국과학기술연구원(KIST) 연료전지연구센터

태양광 또는 전기 에너지를 이용하여 전기화학적 물분해를 통해서 수소를 생산하고 이를 연료전지 등에 활용하는 것은 향후 수소를 기반으로 하는 경제산업 구조를 이루기 위해서 매우 중요하다. 광전기화학을 통한 물분해 연구는 지속가능한 수소생산을 위해서 지난 40 여년간 널리 연구되고 있다. 인공광합성 물분해에 필요한 양성자 환원과 물 산화반응이 잘 일어나기 위해서는 i) 광에너지을 흡수하기 위한 광전기화학촉매, ii) 광촉매 표면에서 화학반응의 활성화 에너지를 낮추는 전기화학촉매 등이 필요하며, 이를 효과적으로 이용할 수 있는 전극 구조와 광화학 반응기도 필요하다. 본 발표에서는 인공광합성 반응의 한 분야인 물분해 수소생산을 중심으로 광전기화학 반응의 각 요소가 가지고 있어야 하는 성질과 광전기화학 수전해의 최근 연구 동향에 대해서 간략하게 논의하고자 한다. 또한 주사전기화학현미경(Scanning Electrochemical Microscopy)을 이용하여 도체 및 반도체 전극 위에서 광촉매 또는 수전해 촉매를 분석하는 실험을 소개한다. 주사전기화학현미경은 물산화반응 중에 생성되는 수산화 라디컬의 농도를 적정하거나 물산화반응의 패러데이 효율을 측정하는 등 다양한 전극 표면의 성질이나 반응의 전기화학 분석을 가능하게 해준다. 덧붙여, 수소저장화합물의 탈수소화 반응을 통하여 수소를 생산하는데 광촉매를 활용할 수 있는 가능성도 살펴본다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC2-2**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry Ⅱ
발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 장진호

Electrodeposited 3-dimensional porous architectures for next-generation lithium batteries

석정돈

한국화학연구원 차세대전지소재연구그룹

Applications of energy storage in transportation and grid scale call for next generation of batteries with high energy and power, good rate capability, long cycle life, good safety and low cost. The development of nanotechnology in the past two decades has generated great capability of controlling materials at the nanometer scale and the creation of nanostructured electrode materials represents one of the most attractive strategies to dramatically enhance battery performanceOur research focuses on the development of electrochemical approaches for the manufacturing of 3D porous nanostructured anodes for Li-ion batteries and cathodes for Li-air batteries. We developed 3D porous silicon anodes for Li-ion batteries by an electrodeposition method using two types of templates such as hydrogen gas bubble template and inverse opal template. Moreover, we developed carbon free, noble metal nano-catalysts coated on 3D porous metal cathodes by a simple electrodeposition method for Li-air batteries. Compared with chemical vapor deposition or etching method for 3D porous nanostructured electrode, electrodeposition method is a simple and low-cost method which is used for large scale operation in industry. The great performance using the 3D porous nanostructured electrodes represents a promising approach for high-performance electrodes which are compatible with scaled-up manufacturing process for next-generation batteries due to their simple and rapid fabrication process.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC2-3**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry Ⅱ
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 장진호

Fabrication and electrochemical applications of a micro-gap electrode

박준희

전북대학교 화학교육과

Large-area micro-gap electrodes were fabricated employing uniform-sized spherical beads as spacers to precisely control the gap thickness ranging from 500 nm to 8 µm for large amperometric signal by the combination of electrochemical amplification by redox cycling and the large area of the electrodes. As a biosensor application, dopamine oxidation with an Au–Au (4 µm) gap showed selective and sensitive amplification of dopamine in the presence of ascorbic acid.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC2-4**
발표분야: New Frontiers in Electrochemistry: Physical and Analytical Electrochemistry, Electrocatalysis, and Photoelectrochemistry Ⅱ
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 장진호

Anti-Galvanic Reduction of Silver Ion on Au and Its Role in the Growth of Anisotropic Au Nanomaterials

황성필

고려대학교 신소재화학과

The role of silver ions in the seed-mediated growth of gold nanostructures has been investigated. Silver submonolayer or monolayer on specific facet of gold is assumed in previously suggested mechanism owing to underpotential deposition (UPD) of silver by ascorbic acid having weak reducing power. Silver overpotential deposition by ascorbic acid, however, is confirmed by electrochemical stripping voltammetry, whereas submonolayer of silver on gold is spontaneously formed by anti-galvanic reduction in the absence of ascorbic acid. In the presence of cetyltrimethylammonium bromide (CTAB), silver overpotential deposition by ascorbic acid does not occur but submonolayer of silver is formed on gold surface. Adsorption of silver and CTAB on gold dramatically hindered the electron transfer by the oxidation of ascorbic acid on gold, which reduces gold ions to metallic gold in seed-mediated growth. These results provide the evidence to the in-depth observation of mechanism in seed-mediated growth where the blocking effect on CTAB/Ag(submonolayer)/Au for oxidation of reducing agent determine the shape and facet of gold nanomaterials.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC-1**
발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 강석진

화학교수학습상황에서 모델링 기반 수업전략에 대한 탐색

강여은 이동원[1,*] 남정희[2]

부산대학교 교육대학원 [1]KAIST 과학영재교육연구원 [2]부산대학교 화학교육과

모델은 대상이 가지는 특징들을 나타내기 위해 대상을 단순화시킨 표현이다. 모델을 통해 학습자는 관심 있는 대상이나 현상에 대해 설명이나 예측을 할 수 있으며, 보이지 않은 대상에 대해 시각적인 표현이나 개념에 대한 구조를 제시함으로써 실제와 이론을 연결할 수 있다. 이러한 모델이 가지는 이러한 특성을 교육에 활용하고자 하는 움직임이 나타나고 있다. 그러나 교육과정에서 모델링이 가지는 중요성에 비해 실제 수업에 모델링을 적용하는 교사가 가지고 있는 모델에 대한 이해는 차이가 있다. 따라서 이를 효과적으로 수업에 적용하기 위한 모델과 모델링의 본성과 전략에 대한 이해는 앞으로 교육현장에 서게 될 예비 교사들에게도 동일하게 요구된다.이 연구에서는 예비과학교사들의 모델형성 능력을 알아보기 위해 논의 기반 일반화학에서 예비과학교사들이 제시하는 모델의 수준을 분석하고 모델형성 능력의 변화과정을 탐색하고자 하였다. 모델형성 능력을 알아보기 위해서 예비과학교사들이 제시하는 모델을 분석하였으며, 모델형성 능력의 변화과정에 대한 이유를 탐색하기 위해 인터뷰를 실시하였다. 이를 위해 일반화학을 수강하는 사범대학 화학교육과 1 학년에 재학 중인 예비과학교사 21 명을 대상으로 11 개 주제의 논의 기반 일반화학 실험 프로그램을 적용하여 수업을 진행하였다. 논의 기반 일반화학 실험수업을 위한 모둠을 구성하기 위해 프로그램의 적용 전 화학개념검사를 실시하였으며, 검사결과를 토대로 화학 II 과목의 수강 여부를 고려하여 이질적인 모둠을 구성하였다. 또한 모델링 능력의 변화 과정을 고찰하기 위해서 모델의 요소, 모델링 전략, 모델링 수행 상의 어려움 및 해소방안에 대한 주제로 인터뷰를 실시하였다. 모델링 단계에서 예비과학교사들의 모델형성 능력을 알아보기 위해서 예비과학교사들이 제시하는 모델의 수준을 분석하였다. 모델의 수준을 분석하기 위한 분석항목은 설명영역, 비교영역, 추상영역, 표식영역의 총 4 가지 항목으로 구분하였으며, 0 수준, 1 수준, 2 수준, 3 수준으로 나누어 분석하였다. 논의 기반

일반화학 실험과정 후 작성하는 결과보고서의 모델링 단계를 분석한 결과, 예비과학교사들의 모델형성 능력은 설명영역, 비교영역, 추상영역, 표식영역 전반에 걸쳐 모델링 단계를 경험함에 따라 점차 향상되는 경향을 보였다.모델형성 능력 변화의 이유를 탐색하기 위한 인터뷰를 분석한 결과, 모델의 요소에 대해 자신만의 모델링 지식을 가지고 모델링 단계를 작성한 예비교사들의 모델형성능력이 설명영역, 비교영역, 추상영역, 표식영역에서 골고루 향상 되었다는 것을 알 수 있다. 특히 수준 높은 모델링 지식에 해당하는 메타모델링 지식의 습득 여부를 알 수 있는 모델링 전략에 대한 질문을 통해 다른 사람의 이해 수준을 고려하여 모델을 의사소통의 수단으로써 사용한 예비과학교사들이 제시하는 모델의 메타모델링 수준이 높게 나타남을 알 수 있었다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **EDEC-2**

발표분야: Current Trends in Chemistry Education

발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 강석진

초등학교용 교과 중심 융합인재교육 프로그램의 개발 및 적용

공영태

진주교육대학교 과학교육과

연구는 교과 중심 융합인재교육 프로그램을 현장에 적용하여 통합적 접근에 대한 이해를 넓히고 과학적 소양을 함양을 위한 학습지도에 시사점을 얻기 위하여 융합인재교육(STEAM)을 적용한 과학 수업이 초등학생의 과학 학습 동기, 과학에 관련된 태도 및 자기 효능감에 미치는 영향을 알아봄으로써 재구성한 과학수업이 현장에서 실효성이 있는지 알아보려 한다. 이 연구에서는 융합인재교육(STEAM)에 적합하도록 6 학년 1 학기 1 단원 '빛'의 4 차시 수업과 2 단원 '산과 염기'의 6 차시 수업을 재구성하여 초등 과학 수업에 적용하고 어떤 효과가 있는지 살펴보았다. 연구대상은 경남 S 시에 소재한 S 초등학교 6 학년 학생들을 대상으로 실시하였다. 그 중에서 2 개 반은 융합인재교육(STEAM)을 적용한 과학수업을 하지 않은 비교반으로, 나머지 1 개 반은 융합인재교육(STEAM)을 적용한 과학수업을 한 실험반으로 선정하였다. 이번 연구에서는 다음과 같은 결론을 얻을 수 있었다. 첫째, 융합인재교육(STEAM)을 적용한 과학 수업은 초등학생의 과학 학습 동기에 유의미한 효과가 있었다. 이는 생활 주변의 현상을 바탕으로 '왜 그럴까'라는 생각에서 출발하는 상황제시 단계를 거쳐 학생들이 창의적으로 설계하여 직접적으로 조작하고 만드는 활동을 통하여 스스로 문제를 해결하였다는 자신감과 성취감을 맛보는 감성적 체험으로 연결되도록 구성한 프로그램으로 과학 수업에 대한 자신감과 즐거움 제공과 함께 수업에 대한 부담 감소로 학생들의 과학 학습 동기 향상에 긍정적인 영향을 주었을 것으로 여겨진다. 둘째, 융합인재교육(STEAM)을 적용한 과학 수업은 초등학생의 과학에 관련된 태도에 유의미한 효과가 있었다. 융합인재교육(STEAM)을 적용한 과학수업은 다양한 영역이 통합되어 학생들이 주도적으로 할 수 있는 활동이 많이 포함되어 있어 지루하지 않게 학습활동에 참여할 수 있으며 창의적 설계 과정 속에서 흥미를 느끼고 결과물을 통해 성취감과 자신감을 가질 수 있었다. 또한 친구들과의 피드백과 감성적

체험과정을 거치면서 학생들의 과학에 관련된 태도가 많이 향상됨을 확인할 수 있었다. 셋째, 융합인재교육(STEAM)을 적용한 과학 수업은 초등학생의 과학 자기 효능감에 유의미한 효과가 있었다. 본 연구의 융합인재교육을 적용한 과학 수업은 수학이나 기술/공학의 요소가 좀더 정확하게 과학지식을 활용할 수 있게 도움을 주어 학습에서 학생들이 성공을 경험할 수 있도록 해 주었고 이 성공의 경험이 학생들의 자기 효능감에 긍정적인 영향을 주었다. 이러한 결과를 바탕으로 융합인재교육(STEAM)을 적용한 과학수업이 초등학생의 과학 학습 동기, 과학에 관련된 태도 및 자기 효능감에 긍정적인 영향을 미치고 있으며, 과학교과를 기반으로 한 통합적 접근으로서 가치가 있다고 본다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC-3**
발표분야: Current Trends in Chemistry Education
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 강석진

시각장애학생의 과학학습상황 이해하기

김학범 차정호[1,*]

경북대학교 계통진화유전체학연구소 [1]대구대학교 과학교육학부

시각장애학생의 과학교육을 위해서는 이들이 어떤 상황에서 관찰하며 탐구하는지 파악하여 교육 내용과 교수 방법을 결정해야 한다. 이를 위해서는 정안의 교육자가 시각장애학생의 과학학습상황을 어떻게 이해하고 있는지 파악하는 것이 중요하다. 본 심포지움에서는 과학교육자, 특수교사 그리고 예비과학교사에게 암실에서의 과학 활동을 직접 경험하게 하여 시각장애학생의 과학학습상황에 대한 인식을 공유하고자 한다. 시각장애학생의 과학학습상황과 유사한 경험을 제공할 수 있도록 시각적 정보가 완전히 차단된 환경에서의 암실 속 과학탐구 활동을 구성하여 연구 참여자들에게 적용하였다. 참여자들은 암실 안에서 얼음과 눈의 촉각 모형을 개별적으로 탐구하였으며, 이 과정에서 연구자와의 대화 및 토론을 통해 시각장애학생의 과학학습에 대한 자신의 생각을 드러냈다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

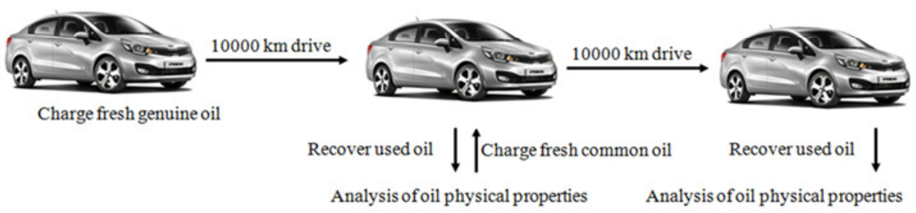
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR-1**
발표분야: Advances in Chemisty of Energy
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 김동욱

Comparison Evaluation of Distribution Engine Oil in Korea

임영관

한국석유관리원 석유기술연구소

Domestic vehicle companies have been selling genuine engine oil with higher price than same grade of regular engine oil. In this study, our group had investigated the properties of engine oil for 14 kinds of genuine and equivalent regular engine oil (KS product) species under fresh and used condition which were recovered after 10000 km driving.In analytic results, genuine engine oils had similar physical properties to regular engine oils under fresh condition. But recovered regular engine oils had better properties in lubricity, kinematic viscosity and acid number change than recovered genuine engine oils.



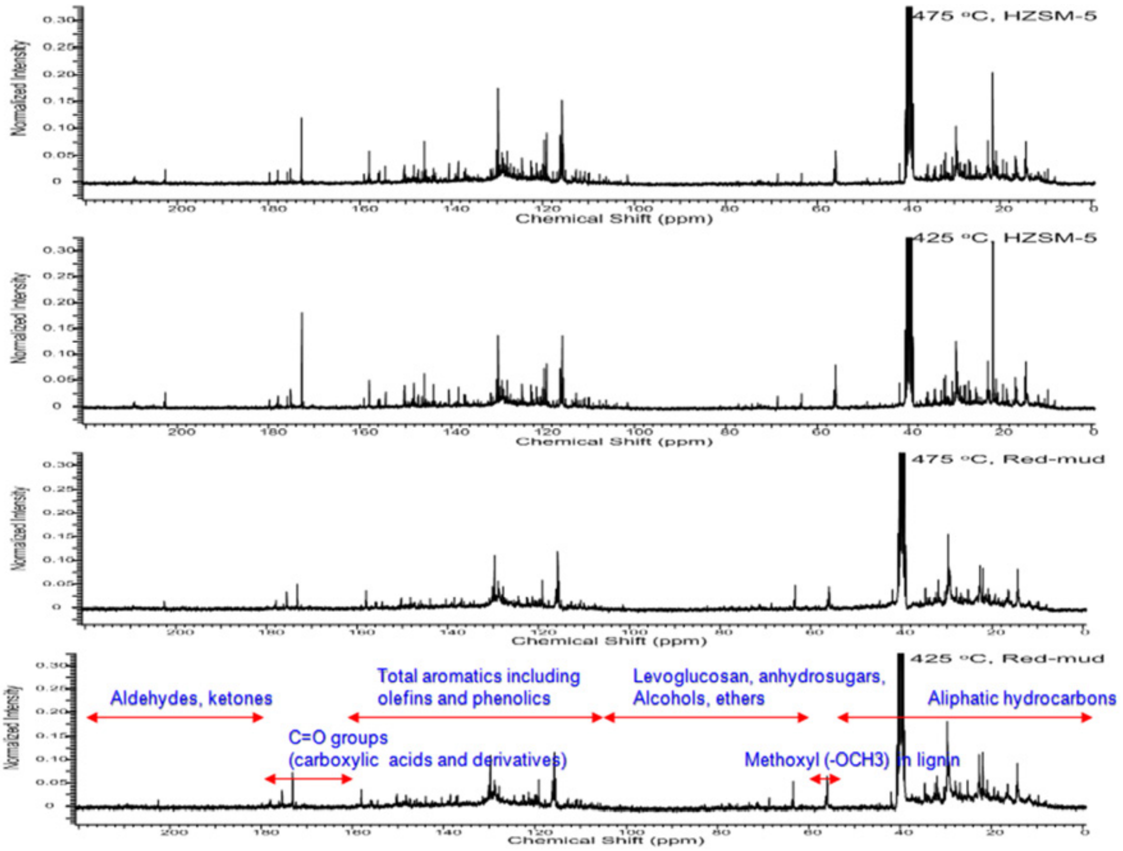
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR-2**
발표분야: Advances in Chemisty of Energy
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김동욱

Production of bio-oil through catalytic pyrolysis of Milkweed

김승수* Foster A. Agblevor[1]

강원대학교 삼척캠퍼스 화학공학과 [1]Utah State University

Fast pyrolysis and catalytic pyrolysis of Milkweed was carried out in a a bubbling fluidized bed reactor. Total liquid yield of Milkweed was between 40.74% and 44.19 wt% at the temperature ranges of 425-550 ℃. The gas yield was increased from 27.90 wt% to 33.33 wt% with increasing reaction temperature. Catalytic pyrolysis of Milkweed with HZSM-5 and Red-mud showed less liquid yield than fast pyrolysis, whereas gas yield was higher than that of fast pyrolysis. The higher heating value (HHV) of the Milkweed bio-oil (organic fraction) showed high values, which were 30.33-32.87 MJ/kg of fast pyrolysis and 35.31~37.23 MJ/kg of catalytic pyrolysis respectivey, with the differences of reaction temperature, feeding rate and fluidization velocity. The selectivity of CO2 was the highest within non-condensable gases, and the molar ration of CO2/CO was about 3 at the different reaction conditions. On product distributions in 13C-NMR analysis, C=O (carboxylic group and derivatives) was higher at 425 ℃ than 475 ℃, which resulted in slightly higher oxygen content in bio-oil. Aliphatic hydrocarbons were slightly higher at 475 ℃ than 425 ℃, and it caused higher pH of aqueous phase.


475 °C, HZSM-5
425 °C, HZSM-5
475 °C, Red-mud
425 °C, Red-mud
Normalized Intensity
0
0.05
0.10
0.15
0.20
0.25
0.30
Chemical Shift (ppm)
200
180
160
140
120
100
80
60
40
20
0
Aldehydes, ketones
C=O groups
(carboxylic acids and derivatives)
Total aromatics including
olefins and phenolics
Levoglucosan, anhydrosugars,
Alcohols, ethers
Methoxyl (-OCH3) in lignin
Aliphatic hydrocarbons

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR-3**
발표분야: Advances in Chemisty of Energy
발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: 김동욱

Engineering Thermoelectric Materials for High Energy Conversion Efficiency from Waste Heat to Electrical Energy

이순일

한국세라믹기술원 에너지환경소재본부/에너지소재센터

It is the nature that thermal energy is absorbed or released in moving of organics and state change of inorganics, indicating that there exist huge thermal resources everywhere. The nature is not a closed system, so every work can be converted into thermal energy, but not reversible according to the second law of thermodynamics. Therefore, a large amount of heat/thermal energy is being wasted in our life, such as body heat, equipment/machine generating heat/thermal energy as a secondary energy or using thermal energy as a primary energy source, and so on. Thermoelectric power generation is a unique technology that can convert the waste heat energy into electrical energy by solid-state energy conversion. Promising thermoelectrics require high electrical conductivity and thermopower and unfortunately low thermal conductivity as well, which makes it difficult to engineer thermoelectric materials due to the correlationship between the electrical conductivity, thermopower, and thermal conductivity in terms of carrier concentration. This seminar will discuss broad aspects in designing and engineering the thermoelectric materials using high-order control of FOM (Figure of Merit).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR-4**
발표분야: Advances in Chemisty of Energy
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 김동욱

Chemical Conversion of Nanoparticles for Electrochemical Energy Applications

하돈형

중앙대학교 융합공학부

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

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **KCS1-1**

발표분야: 대한민국 미래를 위한 기초연구 발전 비전과 2017년도 기초연구사업 설명회

발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 이상기

대한민국 미래를 위한 기초연구 발전 비전

김성규

미래창조과학부 기초연구진흥과

미정

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **KCS1-2**

발표분야: 대한민국 미래를 위한 기초연구 발전 비전과 2017년도 기초연구사업 설명회

발표종류: 심포지엄, 발표일시: 목 11:40, 좌장: 이상기

2017년도 기초연구사업 시행계획 의견 수렴

남계춘

전남대학교 화학과

미정

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS2-1**
발표분야: [IBS 심포지엄] Novel Carbon Chemistry and Materials
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: Christopher W. Bielawski

Lanthanum-catalyzed synthesis of 3D graphene-like ordered microporous carbons in zeolite-template

김경수 유 룡[1,*]

기초과학연구원 나노물질및 화학반응 연구단 [1]기초과학연구원 나노물질및화학반응연구단

In recent years, nanoporous carbons were extensively studied as absorbents, catalytic supports and electrical energy storage electrodes. In particular, ordered mesoporous carbons, synthesized through nanocasting method, attracted much attention due to their regular and three-dimensionally interconnected pore structure with very high specific surface area. Here, we present synthesis of another type of ordered nanoporous carbons with fully graphene-like sp2 carbon framework, using metal ion catalysts (e.g., La^{3+}, Y^{3+} and Ca^{2+}) incorporated within zeolite pores via a simple ion change process. The X-ray crystallographic analysis using zeolite single crystals revealed that a curved graphene-like single layer of carbon atoms was generated along the zeolite pore walls. After removal of the zeolite template in HF-HCl, the resultant carbons exhibited well-ordered microporous structure and high electrical conductivity. We demonstrate that this synthesis approach can be easily scale-up, which is important for various practical application such as absorbents, Li-ion batteries and catalysts.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS2-2**
발표분야: [IBS 심포지엄] Novel Carbon Chemistry and Materials
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: Christopher W. Bielawski

Salty pleasures: High-yielding precursors for doped carbon materials

GOOSSENS KAREL CELE STIJN W[*] **Christopher W. Bielawski**[1,*]

UNIST IBS CMCM [1]*UNIST/IBS CMCM 화학과*

We will demonstrate how suitably designed organic salts may be used as high-yielding precursors for carbon materials via simple thermal treatments. The carbon products are heteroatom-doped, in some instances porous, and/or they show a template-like structure. It is straightforward to tune the heteroatom content and to incorporate metals as well. The materials have been characterized by a range of techniques, including variable-temperature optical microscopy, DSC, TGA, TGA-IR, TGA-MS, elemental analysis, XPS, SEM-EDS, Raman spectromicroscopy and powder X-ray diffraction. We will present the design, synthesis and thermal characteristics of the salt-based starting materials, the structure and properties of the corresponding products that result from thermal treatment, and potential applications of various materials, including their use as electrocatalysts for the oxygen reduction reaction. This work was supported by the IBS (IBS-R019-D1).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS2-3**
발표분야: [IBS 심포지엄] Novel Carbon Chemistry and Materials
발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: Rodney S. Ruoff

Synthesis of polymer precursors for sp^3-bonded carbon materials

이선화 CHEN XIONG Rodney Scott Ruoff[1,*]

기초과학연구원 다차원탄소재료연구단 [1]UNIST 화학과

Diamond, a crystal composed of sp^3-bonded carbon, has high mechanical strength and hardness, high thermal conductivity and chemical stability, and can provide good electrical isolation or when doped can be used for electronic devices. Typical methods for making sp^3-bonded carbon include by applying high temperature and high pressure with metal catalyst(s) to a precursor carbon, or chemical vapor deposition (hot wire or plasma-enhanced) of carbon to make diamond thin films. Another route that we are pursuing is by pyrolysis of organic precursors that can be converted to sp^3-bonded carbon during the heating process. If it were possible to efficiently and in a straightforward way make diamond or carbon materials with high sp^3 content from polymer precursors it could open new avenues for obtaining materials of desired shape.We present preparation of a hyperbranched polymer precursor for sp^3-bonded carbon materials. Hyperbranched polymer precursors have been previously reported and we recently developed a new method that we find effective for making this type of polymer. The effort to convert this polymer into sp^3-bonded carbon was studies. *This work was supported by IBS-R019-D1.*

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS2-4**
발표분야: [IBS 심포지엄] Novel Carbon Chemistry and Materials
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: Rodney S. Ruoff

Leaf-Inspired Highly Efficient and Stable Electro, Photo-catalyst using Hybrid Carbon Nanostructure

정희태

KAIST 생명화학공학과

Photosynthesis in leaves is achieved through unique structural and chemical strategies that ensure high-efficiency energy conversion and long-term stability. The structures of leaf sponge cells scatter light, provide efficient gas diffusion, and enhance molecular adsorption. Chemically, a leaf's unique catalytic system, the Z-scheme, generates photoexcited electrons at each chlorophyll molecule (P680) and transports these electrons via an electron transfer channel (a cytochrome b6f complex) to another chlorophyll (P700) to increase the production yield and selectivity. Here, we designed a highly efficient and stable photocatalyst that drew upon the structural (3D) and systemic advantages (Z-scheme) of natural leaf systems to photoreduce CO2. The photocatalytic activity and CO2 conversion results revealed that the structure and photophysical properties of the system provided synergic improvements in the photocatalytic performances. The artificial Z-scheme with an electron flow from TiO2 via graphene into the few-layered MoS2 could effectively lower the charge recombination rate and increase the potential for CO2 reduction. The TiO2, graphene, and MoS2, all of which are stable and abundant materials, effectively contributed to the stability of the catalyst over many reaction cycles. Our leaf-inspired noble metal-free photocatalyst offers a high CO selectivity of 97% and a high CO production yield (93.22 μmol/g·h) 15 times that of bare TiO2, and is resistant to photodegradation. This artificial leaf presents a new approach to mimicking natural photocatalysts and shows promise as a scalable high-performance non-metal CO2 conversion catalyst.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **KCS3-1**

발표분야: 신종질병 대응기술 포럼

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 박철민

신종감염병 진단을 위한 고감도 진단기술개발

김승일

한국기초과학지원연구원 질환표적기능연구팀

기후 변화와 해외 여행 및 교역의 증가에 따라 신종 바이러스에 의한 감염병 유행의 위험이 커지고 있다. 2015 년 중동에서 유입된 Middle East respiratory syndrome coronavirus (MERS-CoV)의 감염이 확산됨에 따라 186 명의 감염자 및 36 명의 사망자가 발생하였으며 사회 불안을 초래하여 경제적 피해를 20 조원 이상으로 추산하고 있다. 이러한 신종 바이러스의 유입 및 감염 확산을 방지하기 위해 감염원의 신속하고 정확한 진단이 매우 중요하다. 그러나 현재 가장 널리 이용되고 있는 Polymerase chain reaction (PCR) 기반의 분자생물학적 검사법은 시간이 오래 걸리고 진단에 전문인력이 필요한 단점이 있다. 이에 본 연구 그룹은 해외 유입 신종 바이러스에 의한 감염병을 신속하고 정확하게 진단할 수 있는 고감도 진단기술을 개발하고 있다. 이번 세미나에서 누구나 신속하고 간편하게 진단 할 수 있는 현장진단 기술로서 항원-항체 반응 기반 신속진단키트, 매우 높은 민감도로 차세대 진단 기술로 각광받고 있는 나노소재 Field effect transistor (FET)기반 바이오센서, 그리고 페이퍼 센서 개발 기술, 또한 확진 기술로서 나노라만 기반 조기 검출 기술, Next generation sequencing (NGS) 기반 고속진단 기술을 소개하고자 한다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS3-2**
발표분야: 신종질병 대응기술 포럼
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 박철민

Development of mucosal vaccine adjuvants using antigen-targeting strategy to M cells

장용석

전북대학교 분자생물학과

Mucosa-associated lymphoid tissue (MALT) is defined as solitary organized mucosa-associated lymphoid follicles and is subdivided by anatomical region. MALT is characterized as lacking afferent lymphatics, therefore only taking up exogenous antigens through its follicle-associated epithelium, which contains enterocytes, goblet cells, and microfold (M) cells. Among the mucosa-associated lymphoid tissues, the gastrointestinal mucosa maintains a tolerogenic microenvironment to protect the body from unwanted induction of the immune response to continuously exposed commensal microorganisms and food antigens. Considering that 90% of infections occur in mucosal areas, it is conceivable that using mucosal vaccination to establish protective immunity in this frontline of pathogen infection could offer great advantages in current vaccination strategy. However, the number of currently available oral vaccines is very limited compared to the number of parenteral vaccines. This limited availability of oral mucosal vaccines is closely related with the lack of an effective antigen delivery system and a strong adjuvant to stimulate immunity due to the intrinsic nature of the mucosal immune system, which has a low efficiency in antigen delivery into the inductive site and a tendency to induce oral tolerance. We have concentrated our efforts to elaborate efficient antigen delivery system to M cells to establish the strategy for effective oral mucosal vaccine development. Initially, peptide ligands capable of targeting conjugated model antigen into M cells were selected from phage display library panning against in vitro human M-like culture model. We also identified the antigen-targeting ability and mucosal immune-modulating activity of human cathelicidin anti-microbial peptide LL-37.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS3-3**
발표분야: 신종질병 대응기술 포럼
발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 윤창수

호흡기 질환 긴급 확산에 따른 위기상황 대응 전략- 메르스 치료물질 개발MERS-CoV:Opportunity for Drug Discovery in Korea

민지영

한국파스퇴르연구소 호흡기바이러스연구실

Discovery and utilization of small molecule compounds are becoming increasingly important part of basic biological researches. When executed judiciously, screening for and optimization of small molecule hits can provide a powerful tool compound by which the latent biology can be dissected to further our understanding of the biological processes. Moreover, such molecules may become a prime starting point for a full-pledged drug discovery effort, thereby constituting a crucial conduit through which an innovative biological concept is translated into an industrial project toward eventual clinical application. Presented in this talk are innovative phenomic approaches that are not only helping to shed a new light on the discovery of first-in-class compound with novel molecular mechanism of MERS-CoV infection, but also providing a great hope of fighting some of the more devastating outbreak in new ways.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS3-4**
발표분야: 신종질병 대응기술 포럼
발표종류: 심포지엄, 발표일시: 금 10:35, 좌장: 윤창수

신종질병 확산방지를 위한 ICT기반 대응전략

안인성

한국과학기술정보연구원 생명의료예측기술연구실

최근 국제사회는 발달된 교통수단과 여행객들을 통한 국가 간 교류의 증가으로 인하여 지금까지 잘 알려지지 않았던 새로운 종류의 급성 감염병들의 출현이 급증하고 있다. 우리나라의 경우에도 2015 년 중동지역 여행객으로부터 전파된 중동호흡기증후군, 일명 메르스로 인하여 적잖은 인적, 경제적 손실이 발생한 바 있으며, 특히 최근에는 지속되는 이상 고온현상 등으로 인하여 기존에 아열대성 질환으로 알려진 감염병들의 국내 유입 가능성이 높아지고 있다. 본 심포지엄에서는 신종 감염병의 확산방지를 위한 ICT 기반의 대응전략에 대하여 간단히 소개한다. ICT 기반의 대응기술 개발은 기존의 질병발생 사후대처에 치중되어 있던 질병대응 방법과 비교하여, 기계학습을 통한 빅데이터 분석을 통하여 질병의 국내유입 이전에 우리나라의 주변국과 주요 교류대상국들의 질병 발생의 징후를 사전에 감지하고, 다양한 수리 과학적 시뮬레이션 알고리즘 개발을 통하여 우리나라 실정에 최적화된 확산 시나리오를 목표로 한다. 본 발표에서는 미국, 유럽 등 일부 선진국들을 중심으로 시도되고 있는 슈퍼컴퓨팅 자원을 활용한 다양한 질병 예측 시뮬레이션 개발 동향을 소개하고, 향후 융합연구단 사업을 통하여 개발되어야 하는 지능형 확산방지 시뮬레이션 기술의 청사진을 공유하고자 한다.

일시: 2016년 10월 12~14일(수~금) 3 일간

장소: 부산 BEXCO

발표코드: **KCS4-1**

발표분야: 사례로 알아보는 특허 심포지엄 (특허청−물질특허연구회 주관)

발표종류: 심포지엄, 발표일시: 금 09:05, 좌장: 신귀임

특허용어 및 명세서의 구성

방성철

특허청

생소한 특허용어를 설명하고, 명세서의 구성을 논문과 함께 비교함으로써 초임 연구원이 특허제도를 쉽게 이해할 수 있도록 유도함.

일시: 2016년 10월 12~14일(수~금) 3 일간

장소: 부산 BEXCO

발표코드: **KCS4-2**

발표분야: 사례로 알아보는 특허 심포지엄 (특허청−물질특허연구회 주관)

발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 신귀임

선택발명과 진보성

김용

특허청

화합물 발명의 경우 대부분이 선택발명임을 감안하여 선택발명의 명세서 작성 요령을 진보성과 관련하여 설명함.

일시: 2016년 10월 12~14일(수~금) 3 일간

장소: 부산 BEXCO

발표코드: **KCS4-3**

발표분야: 사례로 알아보는 특허 심포지엄 (특허청−물질특허연구회 주관)

발표종류: 심포지엄, 발표일시: 금 10:05, 좌장: 신귀임

의견제출통지서와 대응방안

김종호

특허청

의견제출통지서의 내용을 설명하고 이에 대한 대응 방안을 출원인 입장에서 설명함.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3 일간
장소: 부산 BEXCO
발표코드: **KCS4-4**
발표분야: 사례로 알아보는 특허 심포지엄 (특허청–물질특허연구회 주관)
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 신귀임

특허를 위한 연구노트 작성법

지태훈

한국지식재산전략원

특허 및 국가 R&D 연구과제 획득을 위한 연구 NOTE 작성 사례

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS5-1**
발표분야: 대학원생들을 위한 실험실 안전교육
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 이익모

한국사회의 부조리: 안전문화

-"우리 교수님께도 안전강의를 해 주세요"-

이정학

서울대학교 화학생물공학부

우리나라 안전문화의 수준은 OECD 에서 꼴찌에 가까우나 제자리 걸음을 하고 있으니 답답하기만 하다.

교육기관과 이공계 연구소의 실험실 종사자들의 안전과 건강을 보호할 목적으로 2006 년 "연구실 안전환경 조성법"이 선포되었고, 당시의 과학기술부에 "연구환경안전과"가 신설되었다.
재난 후에 항상 뒤따르는 정부의 엄숙한 선포와는 대조적으로 무관심 속에 방치되는 안전 담당부서는 왜소하다.

2-3 명 학생의 한 학기 등록금 정도이면 전체학생의 안전교육을 시키는데 부족함이 없는데도 예산이 없다는 핑계로 웹에 동영상을 띄어 놓고 효과도 별로 없는 피동적 온라인 교육으로 연구실안전법의 법망을 피해가는 대학이나 연구기관들이 즐비하다.

정보통신, 바이오, 국제화 등과 관련이 있는 각종 연구소, 센터, 국제관, 도서관 등에 기부의 미덕을 펼치는 기부자들은 많으나 유독 안전문화 증진에 기여하고자 하는 기부자는 찾아보기 어렵다.

우리나라 안전문화가 답보상태에 있는 원인과 안전문화를 향상시킬 지름길이 어디에 있는지 살펴보고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **KCS5-2**
발표분야: 대학원생들을 위한 실험실 안전교육
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 이익모

사전유해인자위험분석과 연구실책임자의 역할

이광원

호서대학교 안전보건학과

연구실 안전환경 조성에 관한 법률의 제 7 차 개정을 통해 연구실책임자를 의무적으로 지정·운영토록 하였다. 이는 기존의 연구실안전환경관리자를 주축으로 하는 관리적 안전관리에서 연구실현장중심의 안전관리로 변하는 첫걸음이라고 할 수 있다.

신설된 법 제 5 조의 2(연구실책임자의 지정·운영)를 살펴보면, 연구실책임자는 연구실 내에서 이루어지는 교육 및 연구개발활동의 안전에 관한 책임을 지고, 연구활동종사자를 대상으로 연구실의 유해인자에 대한 교육을 실시해야하며, 연구실에서 수행하는 연구개발활동 등에 대한 사전유해인자위험분석을 실시해야 한다. 이과 같이 연구실책임자는 연구실내에서 활동하는 연구개발활동에 대하여 관리 및 책임이 부여된 것이다. 특히, 사전유해인자위험분석 제도는 연구시에서 수행하는 연구개발활동에 유해인자를 찾아내어 안전하게 수행하기 위한 안전관리방법 및 비상조치계획을 수립하도록 하여, 연구실은 안전하게 관리할 수 있는 기반을 마련하도록 하였다.

이에 본 논문에서는 연구실책임자가 사전유해인자위험분석을 이해하기 쉽게 설명하고 안전관리를 위해 수행해야 하는 역할에 대하여 토론해보고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **KCS5-3**

발표분야: 대학원생들을 위한 실험실 안전교육

발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 이익모

연구실 안전환경 조성에 관한 법률과 연구실 안전

이익모

인하대학교 화학과

연구실 안전환경 조성에 관한 법률(이하 연안법)은 2005 년 4 월에 제정되어 2006 년 3 월부터 이공계 연구실의 안전과 연구활동종사자들의 안전한 연구를 도모하기 위하여 시행되었다.이러한 법률이 제정되고 시행된 배경, 사고 사례 및 통계, 연안법 내용과 연구환경 변화에 따른 개정 내용 등을 살펴 보고 사고 예방 가능성을 논의하고자 한다.또한 최근의 연안법 개정에 반영된 연구책임자의 책임을 살펴보고자 한다.

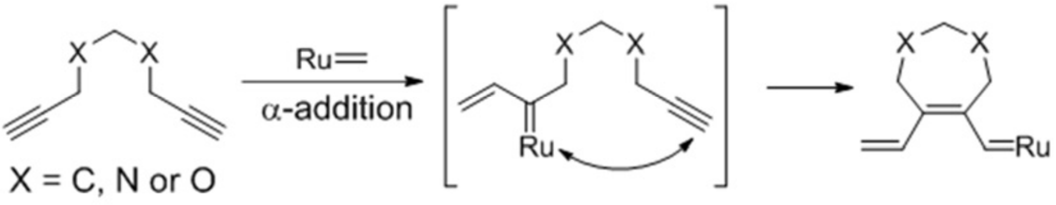
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.O-1**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 고원건

The First Cyclopolymerization of 1,8-Nonadiyne Derivatives

송정아 최태림*

서울대학교 화학부

Diyne derivative 를 이용한 Cyclopolymerization (CP)은 metathesis 반응의 한 종류로 cyclic alkene 을 repeat unit 으로 soluble conjugated polyene 을 만들 수 있는 간단하며 강력한 중합법이다. 지난 50 년 동안 CP 는 1,6-heptadiyne 과 1,7-octadiyne 으로 부터 5 각이나 6 각를 형성하는 연구에 집중되었다. 하지만 alkyne 사이의 거리가 멀어 ring-closing 이 어렵기 때문에 1,8-nonadiyne 의 CP 는 아직까지 보고된 바가 없었다. 우리 group 에서는 1,8-nonadiyne 의 CP 를 위해 1,6-heptadiyne 과 1,7-octadiyne 의 selective α-addition 을 통한 living/controlled CP 를 성공시킨 전략 (Thorpe-Ingold effect 와 짧은 C-N bond 의 도입)과 함께 새로운 전략으로 rotation barrier 가 낮은 aminal 구조와 짧은 C-O bond 를 갖는 acetal 을 도입하였다. 이 monomer 로 우리는 seven-membered ring repeat unit 을 갖는 새로운 polyene 을 합성할 수 있었고 이것은 1,8-nonadiyne CP 의 첫 사례이다. Aminal monomer 는 controlled CP 에도 성공하였으며 mono-alkyne model study 를 통해 선택적으로 α-addition 을 통해 반응이 일어나는 것 또한 알 수 있었다. 이 결과를 통해 CP 로 부터 얻어지는 polyene 의 구조적 다양성을 넓힐 수 있었다.



Cyclopolymerization of 1,8-Nonadiyne Derivatives

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.O-2**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 고원건

Combination of photodynamic therpay and immunotherapy to overcome immunoediting-induced heterogeneity of cancer

임수석 김원종[1,*]

POSTECH IBIO [1]POSTECH 화학과

Recent tendency of cancer therapy is focused on immunotherapy as an alternative method. In spite of its strong anticancer effect, it has been reported that the immunoediting of cancer is an obstacle for successful immunotherapy. Among the pathways of immunoediting, the continuous mutation induces the heterogeneity of cancer, providing with a means of escape from attack of tumor-specific T cells. Therefore, a consecutive release of heterogeneous tumor antigens enables to retain duration of activated immune response and that would be a key factor for successful immunotherapy. Herein, we reported a nanoparticle-based system for combinatorial anticancer therapy by both photodynamic therapy (PDT) and immunotherapy (IT). First, we have fabricated a nanoparticle which can be separated into two nanoparticles under specific condition; one is for PDT and the other for IT respectively. The release of tumor proteins induced by PDT gives increasing chance for dendritic cell to uptake the proteins, presenting on its surface as a tumor-associated antigen (TAA). Moreover, an elongated retention rate of nanoparticle was observed at the tumor site and it is expected that a repetitive PDT helps tumor protein release in a consecutive way. Taken all together, the further investigation is needed to prove long-lasting anticancer immune response via the activation of dendritic cells and CD8+ T cells

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.O-3**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 고원건

How does pyridine stabilize and destabilize the duplex interconnects of spherical nucleic acids (SNAs)?

오주환 이재승*

고려대학교 신소재공학부

Pyridine has been known as a powerful denaturant for duplex DNA for the last 60 years. The duplex destabilization induced by pyridine is attributed to its interactions with nucleobases, leading to a decrease in melting temperature (T_m). Recently, however, pyridine is reported to stabilize duplex DNA under acidic conditions, which needs to be further evaluated and validated using another noble class of polymeric nucleic acids, or spherical nucleic acids (SNAs). SNAs are particularly attractive for the reversible denaturation studies, because they exhibit distinct advantages over conventional nucleic acids, such as sharp melting profiles and distance-dependent optical properties. For the fundamental understading of nucleic acid chemistry with respect to the interactions with heterocyclic aromatic compounds including pyridine, we investigate how pyridine exactly controls the assembly properties of SNAs by eiher stabilizing and destabilizing the duplex interconnects of SNAs. Importantly, we provide highly convincing results demonstrating that a pH change induced by pyridine is crucial to enhance the stability of DNA under acidic condition.

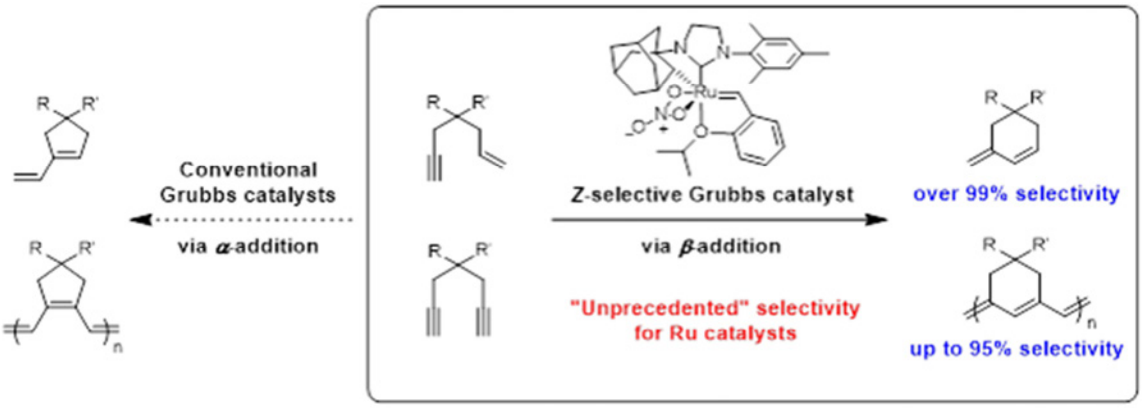
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.O-4**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 고원건

Highly *β*-Selective Cyclopolymerization of 1,6-Heptadiynes Using Grubbs *Z*-Selective Catalyst: Unprecedented Regioselectivity for Ru-Based Catalysts

정기정 최태림*

서울대학교 화학부

It is well known that Ru-based Grubbs catalysts undergo a highly selective *α*-addition to alkynes to promote *exo*-cyclization during ring-closing enyne metathesis (RCEYM) or to produce conjugated polyenes containing five-membered rings during the cyclopolymerization (CP) of 1,6-heptadiynes. There are a few reports of *β*-selective addition to alkynes using Schrock catalysts based on Mo, but none for user-friendly Ru-based catalysts. We report the first example of *β*-selective addition to alkynes using Grubbs *Z*-selective catalyst, which produces only *endo* products during the RCEYM reaction of terminal enynes and promotes the CP of 1,6-heptadiyne derivatives to give conjugated polyenes containing a six-membered ring as a major repeat unit. This unique preference for *β*-selectivity originated from the side-bound approach of alkynes to the catalyst, where the steric hindrance between the chelating N-heterocyclic carbene (NHC) ligand of the catalyst and the alkynes disfavored *α*-addition. To enhance the *β*-selectivity for CP further, one could increase the size of the substrates on the monomers and lower the reaction temperature to obtain conjugated polyenes containing up to 95% six-membered rings. Moreover, the physical properties of the resulting polymer were analyzed in detail and compared with those of the conjugated polyenes containing only five-membered rings prepared from the same monomer, but with a conventional Grubbs catalyst.


Conventional
Grubbs catalysts
via α-addition
Z-selective Grubbs catalyst
via β-addition
"Unprecedented" selectivity
for Ru catalysts
over 99% selectivity
up to 95% selectivity
R
R'
Ru
N
O
n

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.O-5**

발표분야: Oral Presentation for Young Polymer Scientists

발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 고원건

Reactive oxygen species generated by ultrasound stimuli-responsive self-assembled nanoparticle

김선일 김원종*

POSTECH 화학과

In recent years, reactive oxygen species(ROS)-mediated cancer treatment, referred to as photodynamic therapy(PDT), has emerged as a potential alternative because of its minimal invasiveness and improved site-specific action. Many groups, therefore, developed combination system of chemotherapy and photodynamic therapy. However, the non-invasive photodynamic therapy has been limited to treat superficial tumors, primarily ascribed to poor tissue penetration of light as the energy source. Ultrasound can penetrate much deeper in biological tissue because it is non-radiative and has a low tissue attenuation coefficient. The ability of ultrasound to activate some sensitizer such as porphyrin, and 5-aminolevulinic acid has led researchers to consider sonodynamic therapy (SDT) as a possible alternative to PDT. Herein, we designed a ROS stimuli-responsive self-assembled nanoparticle that can be activated by ultrasound to generate ROS. This system has potential of combination of SDT and chemotherapy for cancer treatment.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-1**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 유태수

Sequentially Self-Limited Molecular Layer Deposition of Uniformly Aligned Polyurea Thin Films

박이슬 김혜인[1] 최의진[1] 이진석[1,*]

숙명여자대학교 화학과 [1]숙명여자대학교 화학과

Vapor-phase molecular layer deposition (MLD) is a powerful technique for fabricating conformal ultra-thin organic films with controlled composition and thickness at the molecular level. Although various organic films have been developed over the past two decades using MLD such as polyamide, polyimide, polyurethane, and polyurea, many researchers have focused on MLD growth processes including self-limiting surface reactions and factors that control the film thickness and composition. In order to completely understand the unique properties of organic films, it is necessary to investigate the molecular interaction and orientation in these films in detail.In this talk, we will present uniformly aligned polyurea MLD films by repeating alternative vapor exposures of p-phenylenediisocyanate (PDI) and p-phenylenediamine (PDA) organic precursors for sequential and self-limiting surface reactions on SiO2 substrates. By integrating plane-polarized Fourier-transform infrared (FTIR) and Raman spectroscopic tools, we demonstrated the uniform alignment of polyurea MLD films, which corresponded well with density functional theory (DFT) calculations. Furthermore, the polyurea MLD films were fabricated using different carbon chain length of hydrocarbons, such as ethylenediamine (EDA) and hexamethylenediamine (HDA), to compare the molecular orientations of thin film, which investigated by grazing incidence wide angle X-ray scattering (GIWAXS).

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.O-2**

발표분야: Oral Presentation for Graduate Scholars in Inorganic Division

발표종류: 구두발표, 발표일시: 목 09:10, 좌장: 유태수

Transformation of Coordination Compounds into Functional Nanomaterials

이경주 문회리*

UNIST 화학과

Metal-organic frameworks (MOFs), which are ordered crystalline solids composed of metal clusters and organic linkers, have diverse interesting properties such as structural tenability as well as various functionalities. Recently, the conversion of MOFs as precursors to nanostructured carbon and metal-related materials has attracted increased research interest, caused by their numerous potential applications. The MOF as a precursor possesses a unique advantage that the regular arrangement of metal clusters and ligands in a MOF enables the synthesis of carbon coated metal/metal oxide nanoparticles with highly uniform dispersion and particle sizes. A rich variety of MOF compositions and morphologies also provide the opportunity to prepare the well-tailored nanostructured materials. Although interesting results regarding the synthesis of new materials by the conversion of MOFs have been reported, the fundamental scientific importance of coordination chemistry is not completely understood. Our research is focused on not only the development of synthetic strategy derived from MOF but also the understanding this transformation chemistry. In this talk, we present the novel and simple synthetic strategies that exploit a MOF-derived route towards functional nanomaterials including metal oxide nanomaterials, graphitic carbon, and metal/carbon composites.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-3**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 유태수

A New Type of Polyrotaxane and Self-Catenated Frameworks Based on a Semi-Flexible Dipyridyl Piperazine Linker and a Coligand

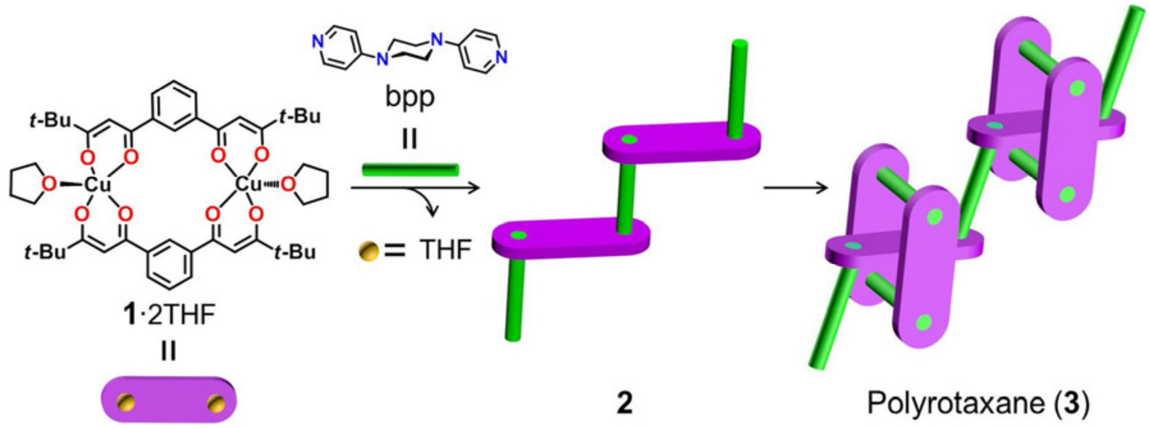
주희영 Jack K. Clegg[1] 박기민[2] Leonard F. Lindoy[3,*] 이심성[*]

경상대학교 화학과 [1]The University of Queensland [2]경상대학교 기초과학연구소 [3]The University of Sydney

In this presentation, we have shown that it is possible to prepare a polyrotaxane motif whose '*string*' and '*bead*' consist of the same components (*see below*).[1] The mixture of planar 'platform-like' complex $[Cu_2(\mathbf{L})_2(THF)_2]$ ($\mathbf{1}\cdot 2THF$)[2] and bpp was refluxed and then slow evaporation of the solution afforded a 1D stair-like coordination polymer $\{(\mathbf{1})(\mu_2\text{-bpp})]\cdot 2THF\}_n$ (**2**). When the reaction solution containing crystals of **2** was left undisturbed for 2 weeks, **2** transformed to the first example of a 1D polyrotaxane $\{[(\mathbf{1})(\mu_2\text{-bpp})][(\mathbf{1})_2(bpp)_2]\cdot bpp\}_n$ (**3**) whose string and bead are made from the same components. On the other hand, the solvothermal reaction of bpp, 4,4′-sulfonyldibenzoic acid (H_2sdb) and divalent metal (Pb or Zn) gave a different structures exhibiting different interlocked topologies.[3] In $[Pb_2(sdb)_2(bpp)]_n$ (**4**), two Pb(II) generate $Pb_2(sdb)_2$ metallacycles connected by bpp ligands, leading to the formation of a 1D + 1D → 1D polyrotaxane. In contrast, in $\{[Zn_2(sdb)_2(bpp)_2]\cdot 2DMA\}_n$ (**5**), tetrameric metallacycles $Zn_4(sdb)_4$ are interlocked, generating 1D polycatenated chains in a parallel manner and are further pillared by bpp ligands to build a 3D framework.

References

1) Ju, H.; Clegg, J. K.; Park, K.-M.; Lindoy, L. F.; Lee, S. S. *J. Am. Chem. Soc.* **2015**, *137*, 9535.
2) Clegg, J. K.; Lindoy, L. F.; McMurtrie, J. C.; Schilter, D. *Dalton Trans.* **2005**, 857.
3) Ju, H.; Lee. E.; Kim, S.; Park, I.-H.; Lee, J.-H.; Lee, S. S. *CrystEngComm* **2016**, *18*, 2621.


N
N
N
N
bpp
t-Bu
t-Bu
O
O
O
O
Cu
Cu
O
O
O
O
O
O
t-Bu
t-Bu
= THF
1·2THF
2
Polyrotaxane (3)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.O-4**

발표분야: Oral Presentation for Graduate Scholars in Inorganic Division

발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 유태수

Investigation of thermal transformation of AuCu alloy nanocrystals embedded in SiO2 shell during thermal oxidation

전기완 이인수*

POSTECH 화학과

Thermal transformation behavior of AuCu-random alloy nanocrystals (NCs) encapsulated by SiO2 shell was investigated by thermal oxidation. The oxidized AuCu NCs were transformed into either Au@CuO core@shell or Au/CuO heterodimer structure. The final morphology of the oxidized AuCu NCs was determined by modulating both annealing temperature in air and Cu content. Au@CuO core@shell structure was produced by either relatively low heat-treatment (150 °C) in air with thick CuO shell thickness or thin CuO shell thickness (a couple of CuO atomic layer) even at relatively high heat-treatment (500 °C) in air. On the other hand, Au/CuO heterodimer was only generated in case of relatively high heat-treatment (> 250 °C) in air with thick CuO shell thickness. During transformation of AuCu NCs into Au/CuO heterodimer, it was found that Au core was migrated toward SiO2 shell as well as migratory behavior of Au core was largely influenced by the CuO shell thickness. By taking advantage of the solid-state protocol for silica-mold nanocrystal conversion, it can provide a general protocol of in-depth study for the conversion of various hybrid nanocrystals and allow to better understand conversion chemistry.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-5**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 유태수

Synthesis of Novel Titanium (IV) Complexes with Tridentate [ONO]-type Ligand and their Usage as Catalysts for Cycloaddition of CO2 to Epoxides

김혜진 현경림 김영조*

충북대학교 화학과

The facile and exclusive synthesis of dimeric titanium (IV) complex with a terminal Ti=O moiety from reaction between novel pyridine-based tridentate ligand(LH2) and Ti(O-i-Pr)4 under the bubbling of wet air is presented. On the other hand, the same dimeric Ti complex was obtained via wet air bubbling of monomeric LTi(O-i-Pr)2 or addition of the same equiv of H2O into LTi(O-i-Pr)2. All compounds including LH2 and two titanium complexes were characterized by single crystal X-ray analyses. Synthesized terminal oxo-titanium compound is the first example of structurally characterized dimeric terminal oxo-titanium compound with no Ti=O→Ti bonds. We will also report two titanium complexes could be used as effective catalysts for the cycloaddition of CO2 to propylene oxide in the presence of various kinds of cocatalysts.Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-6**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 유태수

Designing Crystalline Porous Materials: from Organic Cages to MOFs

김영훈 홍순상 ROHMAN MOHAMMAD RUMUM[1] BENKE BAHIRU PUNJA[1] 고영호[2] 이은성 김기문[*]

POSTECH 화학과 [1]기초과학연구원 복잡계 자기조립 연구단 [2]기초과학연구원 복잡계자기조립연구단

Crystalline porous materials have attracted considerable attention in recent years owing to their potential applications in gas storage, separation and many other areas. We recently reported the synthesis of "porphyrin boxes", porous organic cages with a rhombicuboctahedron-like geometry and permanent porosity, which were rationally designed and synthesized by a combination of well-defined and rigid 3-connected triangular and 4-connected square-shaped building blocks.[1] We envisioned that matallated porphyrin boxes can be utilized as a building block to generate metal-organic frameworks (MOFs) with many exciting potential applications. Indeed, using different lengths and shapes of pillar linkers we have successfully synthesized MOFs with various structures from the molecular organic cages. Details of the work will be presented.

[1] Hong, S.; Rohman, M. R.; Jia, J.; Kim, Y.; Moon, D.; Kim, Y.; Ko, Y. H.; Lee, E.; Kim, K. *Angew. Chem. Int. Ed.* 2015, *54*, 13241-13244.

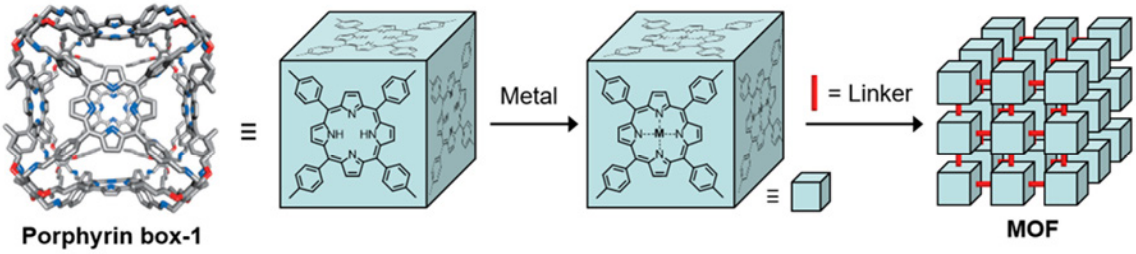


Figure 1. A new approach for construction of MOFs.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.O-7**

발표분야: Oral Presentation for Graduate Scholars in Inorganic Division

발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 박강현

Synthesis of Donor-functionalized Alkoxide Indium Complexes as Precursors for Chemical Vapor Deposition of In_2O_3 Thin Films

정은애 정택모[1,*] 박보근[1] 김창균 손성욱[2]

한국화학연구원 화학소재연구본부 [1]한국화학연구원 화학소재연구본부 박막재료연구센터 [2]성균관대학교 화학과

Indium oxide (In_2O_3) thin films are conductive, transparent to visible light with wide band gap (Eg = 3.7eV) and are used as transparent conducting oxide (TCO) such as ZnO, In_2O_3, GaO_3 and their alloys InZnO, InGaO, and InGaZnO have important applications in the field of opto-electronics, flexible and transparent electronics, digital flat panel display technologies and gas sensors. They exhibit excellent properties such as high mobility, high optical transparency and good environmental stabilities.Indium oxide thin films have been deposited using a variety of methods including sol-gel, sputtering, atomic layer deposition (ALD), physical and chemical vapor deposition (CVD).Several indium precursors for indium oxide film have been studied such as indium acetylacetate [$In(acac)_3$], indium-tris-guanidinates [$In(iPr_2CNR_2)_3$], cyclopentadienyl indium, and trimethylindium (TMIn). All of these precursors are solid, which have disadvantages of low vapor pressure and poor reproducibility, although some of them readily volatilize with mild heating.In this talk, we will display our research results on the synthesis and characterization of novel indium complexes using the functionalized alkoxide as ligands. The molecular structures of complexes have been obtained by single crystal X-ray diffraction studies. The complexes have dimeric configuration with bridging of two alkoxide oxygen atoms between the metals, where indium metal centers in these complexes exhibit penta-coordination state with distorted trigonal bipyramidal geometry. All of the complexes were characterized using FT- NMR, FT-IR, elemental analyses and thermogravimetric (TG) analyses. In_2O_3 films were deposited using new indium precursor by the CVD method.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-8**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 10:10, 좌장: 박강현

CTF-based heterogenized Al-Co bimetallic catalyst for the ring-expansion carbonylation of epoxide to *β*-lactone

<u>R.SENKUTTUVAN</u> PIAO LONGHAI[1] 박규순[*] 윤성호[2,*]

국민대학교 화학과 [1]공주대학교 화학과 [2]국민대학교 생명나노화학과

β-lactone is an important class of intermediates for the ring-opening polymerization to poly(*β*-hydroxyalkanoates), a class of biodegradable and biocompatible polyesters[2]. Although an efficient catalytic system has been reported for conversion of epoxide to lactone[3], a easy way to separate the product and recycling the catalyst is essential for industrial process. Such execution can be attained by replacing homogeneous catalyst with heterogeneous system. The $[\text{bpy-CTF-Al(OTf)}_2][\text{Co(CO)}_4]$ heterogeneous catalyst has been synthesized for the first time by immobilization of $[\text{Al(OTf)}_2]^+$ and $[\text{Co(CO)}_4]^-$ ions into the covalent triazine frameworks (CTFs). The heterogenized catalyst has been characterized using various spectroscopic techniques including Brunauer-Emmett-Teller (BET) surface area, pore size distribution, inductively coupled optical emission spectroscopy (ICP-OES), X-ray photoelectron spectroscopy (XPS) and IR spectroscopy. This heterogenized catalyst efficiently catalyzes the propylene oxide (PO) to *β*-lactone with over 90% selectivity, which is the highest value reported to date. The catalyst can be separated from the reaction mixture by simple filtration and recycled three times while maintaining 70% selectivity in each run, which makes it most attractive for industrial applications.

Acknowledgement: C1 Gas Refinery Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (2015M3D3A1A01064879).

Reference:

1. Sudesh, K.; Abe, H.; Doi, Y. Prog. Polym. Sci. 2000, 25, 1503-1555.
2. Gerngross, T. U.; Slater, S. C. Sci. Am. 2000, 283(2), 36-41.

3. (a) Getzler, Y. D. Y. L.; Mahadevan, V.; Lobkovsky, E. B.; Coates, G. W. J. Am. Chem. Soc. 2002, 124, 1174-1175. (b) Kramer, J. W.; Lobkovsky, E. B.; Coates, G. W. Org. Lett. 2006, 8, 3709-3712.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.O-9**

발표분야: Oral Presentation for Graduate Scholars in Inorganic Division

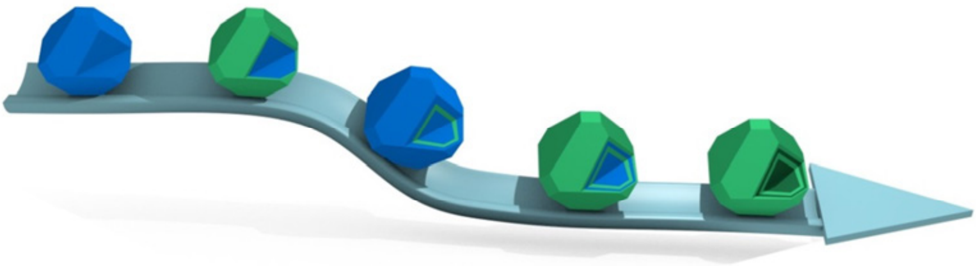
발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 박강현

Evolution Form in Metal-Organic Frameworks: From Metal-Organic polyhedra to Double-shelled Hollow Metal-Organic Frameworks

이지영 최원영*

UNIST 화학과

Making complex forms of micro-/nanostructure has been proposed to control the property of materials. However, compared to development of various exterior architectures in metal and metal oxide systems, it is greatly challenging to synthesize those for porous material, especially metal-organic frameworks (MOFs). Herein, we demonstrate a novel synthetic strategy for double-shelled hollow MOFs via sequential self-assembly. Moreover, this new strategy also allows the various forms, including core-shell, matryoshka and single-shelled hollow MOFs. We anticipate that this synthetic approach will open a new way for development of diverse forms of MOFs together with target application, such as drug delivery/releasing, guest molecule storage and heterogeneous catalytic property.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-10**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 박강현

Direct Self-assembly of Cube-shaped Porphyrin Single Crystal by Reverse Modified Anti-solvent Crystallization method in Binary Solvent System

박요환 임현섭[1,*] 최희철[*]

POSTECH 화학과, 기초과학연구원 CALDES [1]UNIST IBS 다차원 탄소연구단

Among various functional materials, porphyrin-based coordination polymers (PCPs) have attracted significant attention in this respect owing to their morphology–dependent properties including luminescence, light harvesting, and photo-catalysis. Depending on the intermolecular interaction, such as hydrogen bonding, π–π stacking, metal coordination and electrostatic interactions, a lot of porphyrin-based coordination polymers have been fabricated. The PCPs crystallization greatly affected by the addition of surfactants, which facilitate to minimize certain surface energy for growth of crystal into specific plane. However, it remains challenging to fabricate well-defined PCPs without any additive such as surfactant or acid. Here we report a new approach to fabricate high crystalline PCPs via reverse modified anti-solvent crystallization (RM-ASC) method. We synthesized well-defined cube-shaped crystal of zinc 5,10,15,20-tetra(4-pyridyl)-21H,23H-porphyrin (ZnTPyP) using RM-ASC method. Among various solution-phase crystallization methods, anti-solvent crystallization (ASC) is the most widely used solvent-phase method, which can control the environment of the solution by forming binary solvent system. However, local environment control in ASC method has been not studied so far, thus, we demonstrate to control local environment of solute by introducing RM-ASC method and suggest the effect of solvation shell to crystal growth direction. Our approach reveals a noble chemical route to achieve the shape-controlled ZnTPyP cube-shaped crystals by controlling of the solvated molecule, which will extend the synthetic opportunity even for the other organic crystals.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.O-11**

발표분야: Oral Presentation for Graduate Scholars in Inorganic Division

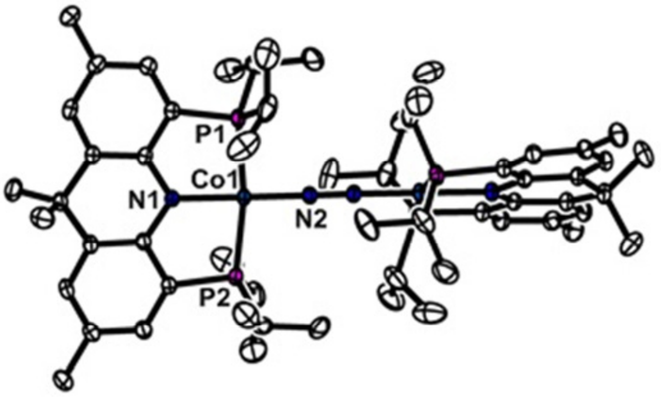
발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 박강현

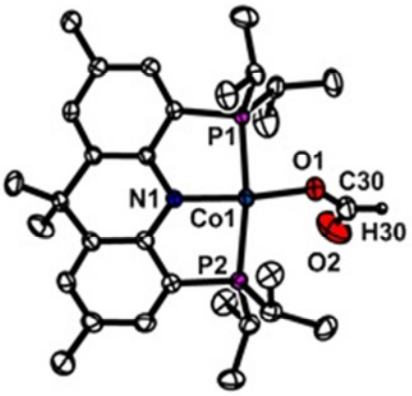
Hydrogenation of CO_2 Catalyzed by PNP Cobalt Complexes

최종훈 이윤호*

KAIST 화학과

A metal-hydride bond is considered as a key moiety for various catalytic organic syntheses. Especially, many rare-earth metal hydride species have been utilized for catalytic CO_2 hydrogenation. Recently, earth abundant 1st-row transition metal complexes have been highlighted due to the cost effectiveness and environmentally benign impact. Development of efficient catalyst is obviously desirable with its appropriate economical merit. Recently, 5- or 6-coordinated 1st-row transition metal complexes have been studied revealing modest catalytic efficiency even at high temperature and high pressure of CO_2. The proper catalyst design is currently demanded to achieve the reasonable efficiency.Here, we will present syntheses and characterization of two series of cobalt complexes supported by two anionic PNP ligands; PNP^- = bis(2-(diisopropylphosphino)-4-methylphenyl)amide and acridane adapted PNP'^- = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide. The PNP ligands can accommodate a metal center in a square planar geometry in the presence of the fourth ligand. A dinuclear cobalt(I) dinitrogen species $\{(PNP)Co\}_2(\mu\text{-}N_2)$ and $\{(PNP')Co\}_2(\mu\text{-}N_2)$ were prepared from the chemical reduction of (PNP)CoBr and (PNP')CoBr, respectively. Upon addition of H_2(g) to a monovalent cobalt dinitrogen species, a corresponding cobalt monohydride species was generated. Further reaction with CO_2(g) produces a cobalt formate species with good yield. Under mild conditions, formate generation catalyzed by $\{(PNP')Co\}_2(\mu\text{-}N_2)$ reveals high TOF of 1900 h^{-1}. Further investigations including the mechanism of formate generation will be discussed in detail.


P1
Co1
N1
N2
P2


P1
O1
C30
N1
Co1
H30
P2
O2

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.O-12**
발표분야: Oral Presentation for Graduate Scholars in Inorganic Division
발표종류: 구두발표, 발표일시: 목 10:50, 좌장: 박강현

Pd Catalysts Supported on N-doped Carbon : Formic Acid Based Hydrogen Storage

한다정 최수빈[1] 박현서[2] 윤창원[2,*]

고려대학교 화학과 [1]경희대학교 KHU-KIST 융합과학기술학과 [2]한국과학기술연구원(KIST) 연료전지연구센터

Abstract Formic acid has been recognized as one of the most promising chemical hydrogen storage materials further applicable to large-scale energy storage systems. Herein, we presented the synthesis and characterization of a scalable Pd catalyst supported on nitrogen doped carbon(N-C) via a simple pyrolysis(550 ℃) using precursors containing Pd, N, and C atoms. Compared to Pd/C, the resulting Pd/N-C catalyst demonstrated the enhancement in catalytic activity for the dehydrogenation of formic acid via the activation of C-H bonds in H-COOH. The increased activity for Pd/N-C was found to originate from electronic interaction between the incorporated nitrogen atoms and Pd active sites, as evidenced by X-ray photoelectron spectroscopy(XPS). Ultimately, a hydrogen generation system fueled by formic acid was designed and further integrated with a polymer electrolyte membrane fuel cell (PEMFC), demonstrating continuous production of the 180 W power over 1h. Keywords: Pd-N-C, Formic acid, Dehydrogenation, Nitorgen doping, Palladium catalyst, PEMFC

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-1**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 김중한

Semiclassical simulations and two-dimensional electronic spectra for understanding photosynthetic energy transfer processes

김현우* 이영민[1,*]

한국화학연구원 화학시뮬레이션센터 [1]POSTECH 화학과

Natural photosynthesis begins with excitation energy transfers from light-harvesting complexes to the reaction center. These processes have been investigated with various experimental methods such as two-dimensional electronic spectroscopy. In the theory community, the detailed mechanism of photosynthesis has been studied by simulating excited-state dynamics on multiple potential energy surfaces of the involved systems. For describing excited-state dynamics in such complex systems, mixed quantum-classical (MQC) approaches have been established based on a partition scheme that divides the whole system into the system of interest and the bath. In these MQC approaches, the system is treated with quantum mechanics while the bath is described with classical mechanics. Here, we present a simulation scheme for generating two-dimensional electronic spectra with an MQC approach, the Poisson bracket mapping equation (PBME). We find that PBME is as reliable as a more accurate method in simulating two-dimensional electronic spectra of simple two-state model systems. We will also discuss the applicability of our scheme to more realistic models of natural photosynthetic pigment-protein complexes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-2**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 09:10, 좌장: 김중한

Conformational relaxation and kinetics of a polymer translocation into a capsid: a Langevin dynamics simulation study

이슬기 성봉준[*] 김준수[1,*]

서강대학교 화학과 [1]이화여자대학교 화학나노과학과

The translocation of a viral DNA into a small capsid is a critical step in viral infection mechanism. Because the number of conformations of the DNA should be decreased significantly into a compact capsid, the entropic cost during the translocation process should be extremely large. A motor protein located at the capsid mouth, therefore, is required to force the DNA to translocate into the capsid. A recent experiment study showed that the DNA underwent non-equilibrium conformational change depending on how the motor protein was stalled and restarted (Proc. Natl. Acad. Sci. USA.,111, 8349 (2014)). And the stalling step resulted in the heterogeneity of the packaged DNA length under the jamming transition. In this study, we perform Langevin dynamics simulations along with coarse-grained models for the DNA, the capsids, and the motor protein. We control parameters such as the force size, the capsid size and the stall period of the motor protein, and investigate how the DNA would be packaged into the capsid. Our simulations show that depending on the existence of the stalling step and the stall frequency, the packaging efficiencies would be enhanced, i.e., the fraction of monomers packaged inside the capsid increases for a given time. And we also construct a contact probability map for the DNA in order to investigate the conformational dynamics during the translocation process.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-3**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 김중한

Water Dynamics in Cellular like Crowded Environment Correlates with the Transition Pathway of the Crowder

VERMA PRAMOD KUMAR 조민행[1,*]

고려대학교 IBS 분자 분광학 및 동력학 연구단 [1]고려대학교 화학과

Polyethylene glycol (PEG; ─(OCH2CH2)n─) is a unique polymer material with enormous applicability such as ion-exchange membrane, crystal formation of proteins and nucleic acids, edible forms for food or drug coating, water treatment etc. PEG contains both polar ether and nonpolar alkyl group and has flexible structure, non-reactivity, very high water solubility, low toxicity, and biodegradability. All these properties make it an excellent artificial crowding agent that are added to the solution to mimic the cellular environment in vitro. Macromolecular crowding refers to a system where macromolecules occupy large volume fractions of the total available volume while restricting the conformational accessible states of a biomolecules [1]. Crowding not only modifies the protein intermolecular forces by way of entropic, excluded volume effects but also by amplifying complex interactions when hydration water layers overlap within several nanometer distances off the biomolecule surface. Since the perturbation of water by the crowders could have significant implications in cellular environments, where the structural and dynamic correlation lengths may extend beyond the space available from interstitial water, we have focused on water structure and dynamics as well as its significance on the whole molecular systems over a wide concentration range of crowder, PEG.Our findings confirm that the crowding significantly perturb the water structure as well as solute-water partnership. The water dynamics do not change much even in highly crowded environment. However, the hydration water slows down considerably under crowding. The microscopic picture obtained from the experiments provides a clear evidence that the crowder itself undergoes a transition from a relaxed well hydrated conformation to a compact collapsed state. This has been possible by employing two different vibrational probes. One is the OD stretch of HDO that provides information on water structure from the water's point of view. The others are the azido stretch of hydrazoic acid (HN3) and covalently linked azido group of PEG. The former provides information from the dissolved solute's point of view and allows a direct assessment of how water's choice of H-bonding is altered by crowder, while the latter explains how the crowder accommodates itself in the crowded environment. We thus anticipate that studying the properties of such a macromolecular crowding environment can shed light on properties of water inside living organism.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-4**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 김중한

Molecular Dynamics Simulations of Viscosity Evolution of Aqueous Amine CO_2 Capture Solutions: Monoethanolamine versus Piperazine

유택희 Yves Lansac[1] 장윤희[2,*]

GIST 신소재공학부 [1]Université François Rabelais, France [2]DGIST 에너지시스템공학

Chemical absorption of CO_2 by aqueous amine solutions is currently the most mature technology to capture CO_2 from post-combustion flue gases. A density-functional-theory-based fast virtual screening of the CO_2-capture performance has been developed for various aqueous amine solutions such as monoethanolamine (MEA; the standard CO_2 capture solution) and piperazine (PZ; the standard fast-CO_2-absorbing component in high-performance blended amine solutions). An important issue in developing high-performance amine solutions for CO_2 capture is that the viscosity of amine solutions containing PZ increases rapidly with the CO_2 loading. A new design of a fast-CO_2-absorbing component as fast as PZ but not as viscous as PZ is therefore desirable. For this purpose, using molecular dynamics simulations combined with Green-Kudo (GK) and Stokes-Einstein (SE) equations, we compute the transport behavior (viscosity and diffusivity) of aqueous PZ solution as a function of CO_2 loading (0 to 0.5 mol/mol) at different conditions (concentration 5-9 M and temperature 298-313 K) and we compare our findings to the experimental data. The result is compared to those of less problematic solutions such as MEA in order to unveil the microscopic origin of such a rapid viscosity increase of PZ. The calculation indicates that the SE method predicts lower viscosities than the GK method. The CO_2-loading-dependent viscosities calculated with the GK method reproduce the experiments.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-5**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 김중한

Galaxy7TM: a web server for flexible GPCR-ligand docking

이규리 석차옥*

서울대학교 화학부

G-protein-coupled receptors (GPCRs) play important physiological roles related to signal transduction and thus form a major group of drug targets. Prediction of GPCR–ligand complex structures has therefore important implications to drug discovery. With previously available servers, it was only possible to first predict GPCR structures by homology modeling and then perform ligand docking on the model structures. However, model structures generated without explicit consideration of specific ligands of interest can be inaccurate because GPCR structures can be affected by ligand binding. The Galaxy7TM server, freely accessible at http://galaxy.seoklab.org/7TM, improves an input GPCR structure by simultaneous ligand docking and flexible structure refinement using GALAXY methods. The server was benchmarked on a wide set of GPCR model structure and small molecule ligand inputs. It showed better performance in both ligand docking and GPCR structure refinement than commonly used programs AutoDock Vina and Rosetta MPrelax. These programs are well known and publicly available for protein-ligand docking and membrane structure refinement, respectively.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-6**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 김중한

Improvement of AFM lithography system and studying characteristics of nano-indentation AFM lithography

김정환* 전승희[1]

한국기초과학지원연구원 질량분석장비개발팀 [1](주)나노포커스 기술연구소

New nanolithography method such as nano-imprint and atomic force microscopy (AFM) nanolithography has the potential value to be future low-cost techniques for nano-scale patterning and fabrication. Nano-indentation lithography using AFM is promising to create nano-structures owing to the ability of both a precise pattering and an in-situ measurement simultaneously.In this study, we have improved the performance of the XYZ scanner of existing commercial AFM system for nano-indentation. Newly designed scanner shows a better precision and reliability for producing nano-pattern than that of original system. Close loop control of XY scanner provides a minimal distortion of pattern shape created by nano-indentation AFM lithography. The new type of scanner shows an enhanced orthogonality and a low cross-coupling of XY and Z, therefore it provides more accuracy and sophisticated control of AFM tip. We also have upgraded a various tip control algorithm and user interface for editing patterns. We have studied the relationship between a pattern shape and indentation parameters. The characteristics of the unique nano-indentation method and its applications will be discussed in detail.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-7**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 10:10, 좌장: 하정현

High-resolution Emission Spectroscopy of Transient Species Produced by Penning Ionization with Metastable Atom

Keiichi Tanaka

Department of Chemistry, Kyushu University

Electronic transitions of the cations, PN^+, OCS^+, ICN^+, $BrCN^+$, and $ClCN^+$, produced by Penning ionization with metastable He* atom were observed by a high resolution Fourier transform spectrometer. The linear triatomic cations such as OCS^+ and $BrCN^+$ are of great interest, because they are open shell radicals with the 2Pi electronic ground state and the vibronic levels in the v2 bending mode are largely affected by the Renner-Teller effect.Seven vibronic bands of the OCS^+ ion have been observed in the 370 − 500 nm region and assigned to the A2Pi − X2Pi electronic transition. The prominent CO stretch progression bands (v1 = 0 - 2~5) were observed from the vibrational ground state of the A2Pi state. It is because the fast predissociation occurs in the vibrationally excited states of A2Pi due to the interaction with the repulsive 4S state. The CO bond length for A2Pi is much larger (by 0.166 A) than that for X2Pi to accord to the observed band intensities. The spin-orbit interaction constants for A2Pi and X2Pi were determined to be −126.5 and −381.0 cm−1, respectively, consistent with the results by photo dissociation study.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.O-8**
발표분야: Oral Presentation for Young Scholars in Physcial Chemistry
발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 하정현

Analytic Pattern Learning

Kar-Ann Toh

연세대학교 전기전자공학과

"The more relevant patterns at your disposal, the better your decisions will be." - Herbert Simon. We shall begin this talk by a conceptual recall of state-of-the-art learning algorithms such as Linear Regression (LR), Linear Discriminant Analysis (LDA), k-Nearest Neighbors (kNN) and Support Vector Machines (SVM) for pattern classification. Next, several closed-form learning formulations for classification are introduced. In particular, the classification total error rate (TER) and the receiver operating characteristics (ROC) are shown to be optimized in closed-form. Such results not only facilitate efficient batch learning, but also they can be extended to online applications where the learning is convergent according to data arrival. These learning formulations are subsequently shown to be inter-related from the data transformation perspective.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-1**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 하지원

Immuno-nanoplasmonic assay on nanoscale: diffraction-unlimited imaging with TIRS nanoscopy

안수진 이승아[1] 강성호[1,*]

경희대학교 일반대학원 화학과 [1]경희대학교 응용화학과

Immuno-nanoplasmonics were localized on nanoscale substrate along the *x*, *y* coordinates using a total internal reflection scattering (TIRS) nanoscopy. 20-nm silver nanoparticles (nanoplasmonics) and 100-nm gold nanoisland (GNI, substrate) were selected as the plasmon nanoparticles due to their distinct scattering wavelengths as the nature of its size, material, and shape. Individual scattering signals of nanoplasmonics and substrate were selectively detected with the evanescent field layer by wavelength-dependent TIRS using 405 nm and 635 nm lasers, respectively. The centroid of the immuno-nanoplasmonics was localized on the GNI by resolving point spread function on applying 2D Gaussian function. This method showed ultrasensitive quantification with a limit of detection (LOD) of 7.04 zM, which was 100 times lower than detection limits obtained with the previously reported total internal reflection fluorescence detection methods. TIRS nanoscopy was demonstrated to be an effective tool for super-localizing individual protein molecules, interactions in nanoscale regions, and was a reliable method for the effective quantitative detection of disease-related protein molecules as diagnostics.

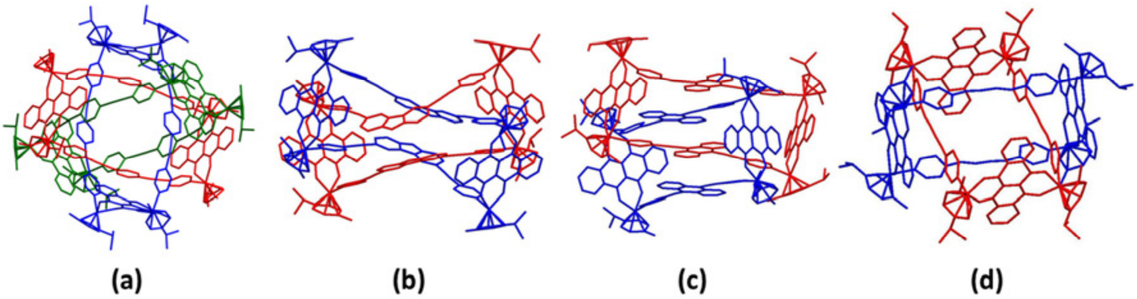
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-2**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:10, 좌장: 하지원

Engineering of Molecular Topology via Coordination-Driven Self-Assembly

SINGH NEM[*] 지기환[*]

울산대학교 화학과

In the past two decades coordination-driven self-assembly has emerged as a well-established method for the rational design of fascinating supramolecular architectures. The self-assembled, threaded molecular architectures such as catenanes, trefoil, and pentafoil knots, Solomon links and Borromean rings have attracted a great deal of attention not only because of their aesthetic charm but also because of their potential applications in nanomaterials, biomaterials, molecular machines, electronic devices, and sensors. Our group has recently used this elegant self-assembly method in realizing rarer molecular topologies such as molecular Borromean rings,[1] Solomon link,[2] Hopf's link[3] and a non-catenane "rectangle-in-rectangle"[4] via suitable modifications in the length, shape, and functionality of the building blocks. Molecular structures of topologies by X-ray crystallography (Figure 1) and solvent, guest-template and concentration effect in solution by 2D ROESY and DOSY NMR will be presented and discussed. Figure 1: X-ray crystal structures of (a) Borromean rings, (b) Solomon link, (c) Hopf's link and (d) a noncatenane "rectangle-in-rectangle" References[1] T. Kim, N. Singh, J. Oh, E. H. Kim, J. Jung, H. Kim, K.-W. Chi, J. Am. Chem. Soc.2016, 138, 8368-8371.[2] Y. H. Song, N. Singh, J. Jung, H. Kim, E. H. Kim, H. K. Cheong, Y. Kim, K.W. Chi Angew. Chem., Int. Ed. 2016, 128, 2007-2011.[3] H. W. Lee, P. Elumalai, N. Singh, H. Kim, S. U. Lee, K. W. Chi, J. Am. Chem. Soc. 2015, 137, 4674-4677.[4] V. Vajpayee, Y. H. Song, T. R. Cook, H. Kim, Y. Lee, P. J. Stang and K.-W. Chi, J. Am. Chem. Soc., 2011, 133, 19646-19649.


(a)
(b)
(c)
(d)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL1.O-3**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 하지원

Preparation of C18 bound silica monolith particles as HPLC stationary phase of improved separation efficiency: Effect of sedimentation on separation efficiency

AliAshraf 정원조*

인하대학교 화학과

Silica monolith particles have been successfully prepared on a large scale by sol-gel process. The particles after calcination were separated by sedimentation into three zones using a plastic-made Imhoff sedimentation cone. The lower zone particles were derivatized with a C18 ligand and end-capped with a mixture of hxamethyldisilazane (HMDS) and trimethylchlorosilane (TMCS). The resultant phase was packed in glass lined stainless steel micro-columns, and the separation efficiencies as high as 150,000 plates /m were achieved for the separation of benzene and its four derivatives. The separation efficiency of this new phase is much better than those of our previous C18 phases and commercial C-18 phase. This study offers a promising vision towards commercialization of chromatographic phases based on silica monolith particles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-4**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 하지원

Multilevel Glycomic Characterization of Protein Therapeutics from Intact Protein to Glycan Analysis

오명진 김운용[1] 서영숙[2] 안현주[2,*]

충남대학교 분석과학대학원 [1]충남대학교 AGRS [2]충남대학교 분석과학기술대학원

The glycosylation pattern of biotherapeutics is considered to be a very important attribute due to itsstrong effect on quality, stability, safety, immunogenicity, pharmacokinetics, and potency. Thus,systematic approach for effective measurement and control of glycosylation from the early stages ofdrug development to post-approval batch release is absolutely required. We have developed stepwisestrategies for glycome quality assessment during drug design and manufacture in the level of intactprotein, glycopeptide, and glycan. For intact protein analysis, C8 Chip-based nano-LC/Q- TOF MS wasemployed for the determination of molecular weight with various glycoforms, glycosylation siteoccupancy, and carbohydrate contents. In-depth site-specific glycosylation with micro & macro glycanheterogeneity can be achieved by glycopeptide analysis which combines molecular size fractionation,multiple proteolysis, PGC nanoLC MS/MS, and in silico screening by accurate mass. Structure-specific and isomer-specific glycan analysis can be done by native glycan analysis using nano LCPGC chip/Q-TOF MS. In terms of glycosylation profiling, we could obtain a result that has a closecorrelation with each other by thee different analytical methods. It is possible to select the analyticalplatform to measure the glycosylation on biotherapeutics based on the required informationthroughout the drug life cycle. This approach could be widely applied for high-quality analyticalcharacterization of glycosylation, starting from early drug development to final lot release.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-5**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 하지원

Corn seed tissue section prepared by tape-support method for mass spectrometry imaging with keeping intact spatial information

김신혜 김정권 이태걸[1] 윤소희[1,*]

충남대학교 화학과 [1]한국표준과학연구원(KRISS) 미래융합기술부

Sample preparation is a crucial step to obtain reliable, high-quality, and intact molecular images of tissue samples for mass spectrometry imaging. A metabolic pathway in biological samples still works in the sample preparation steps. It means molecular composition involved the metabolism may be changed by increasing a temperature or the water content in the tissue, etc. [1] Especially, sample preparation for plant samples is more challenging than animal samples [2]. Plants with high water content are relatively fragile during the cryosection, and thus it makes difficult to obtain intact and thin tissue slices [3]. We suggest a new suitable method in the preparation of the plant tissues for mass spectrometry imaging. The sectioning of the corn seeds was employed using a commercial 3M tape to reduce the distortion of the section surfaces and to exclude the thermal process. The corn seeds embedded in 10% gelatin solution were attached onto 3M tape as adhesive film and then tissue sections were cut at a 10 μm thickness. The sections were slowly freeze-dried using a metal plate chilled below –80 °C in a vacuum desiccator to avoid water condensation onto the tissue surface.In this study, the thermal effect in the sample preparation was demonstrated by time-of-flight secondary ion mass spectrometry (TOF-SIMS) that some molecules were relocalized in the thaw-mounted method. The effect, however, did not be occurred in our method using the tape under the careful temperature controls. There was a significant decrease in sample distortion and re-localization of the molecules within the sample. Also, the contamination on the tissue surface from the gelatin was reduced in comparison with thaw-mounted sample preparation. Details will be discussed in the presentation. 1.Y. J. Lee, D. C. Perdian, Z. Song, E. S. Yeung and B. J. Nikolau, Plant J. 70, 81–95 (2012).2.B. A. Boughton, D. Thinagaran, D. Sarabia, A. Bacic and U. Roessner, Phytochem. Rev. 14, 1–44 (2015).3.S. Cha, H. Zhang, H. I. Ilarslan, E. S. Wurtele, L. Brachova, B. J. Nikolau and E. S. Yeung, Plant J. 55, 348–360 (2008).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-6**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 하지원

Five-dimensional Single Particle Tracking in Live Cells

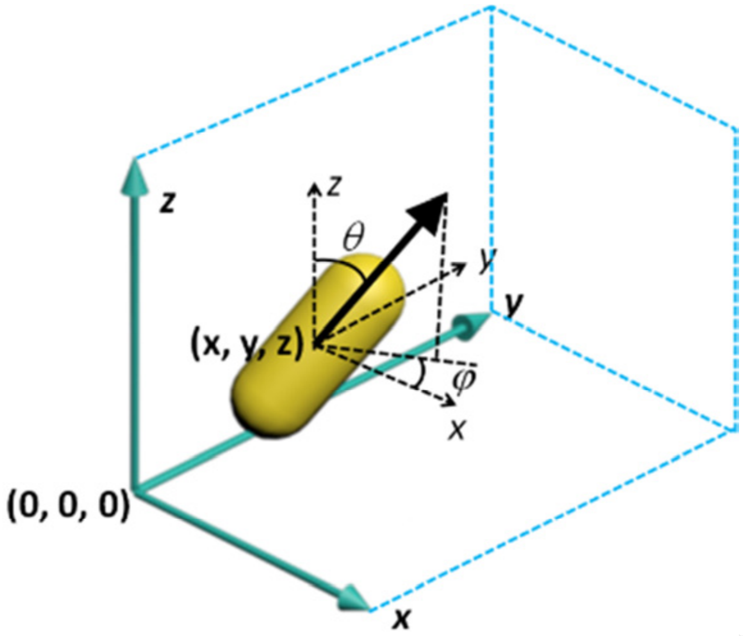
Ning Fang

Associate Professor, Department of Chemistry, Georgia State University, USA

A cell can be conceived as a factory containing a hierarchical network of nanomachines. Fully understanding the working mechanisms of these nanomachines requires knowledge of both translational and rotational dynamics, and their coupling. The knowledge of rotational dynamics in and on live cells remains highly limited due to the limitations of conventional single particle tracking (SPT) techniques and requires further experimental advances through the use of new innovative tools.

The differential interference contrast (DIC) microscopy-based Single Particle Orientation and Rotational Tracking (SPORT) techniques have been developed in the Fang Laboratory to acquire accurate measurements of anisotropic plasmonic gold nanorods in complex cellular environments. Rich information in five dimensions, including the *x, y, z* coordinates and the two orientation angles (azimuthal angle φ and polar angle θ, as defined in the figure) of the probe's transition dipole, can be obtained from SPORT experiments.

The SPORT technique is capable of extracting important information (including rotational rates, modes, and directions) on the characteristic rotational dynamics involved in cellular processes, such as adhesion, endocytosis, and transport of functionalized nanoparticles, as may be relevant to drug delivery and viral entry.


z
z
θ
y
y
(x, y, z)
φ
x
(0, 0, 0)
x

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-7**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:05, 좌장: 하지원

Characterizing Optical Properties of Palladium-coated Single Gold Nanorods

이소영 하지원*

울산대학교 화학과

Gold nanoparticles have received a lot of interest in the last decade because of their unique optical properties, and their potential applications include catalysis, nanophotonics, and bioimaging. Compared to spherical gold nanoparticles, anisotropic-shaped gold nanorods (AuNR) exhibit two localized surface plasmon resonance (LSPR) modes, longitudinal LSPR mode and transverse LSPR mode. The LSPR modes of AuNRs are strongly dependent on size, shape, and the refractive index of surrounding medium. In recent year, core-shell bimetallic nanorods have also received considerable attention because of their distinct photochemical and photophysical properties. The distinct properties are due to synergetic effect of two different metals. Despite the recent progress in the synthesis of core-shell bimetallic nanorods, our understanding on their optical properties is still very limited at the single particle level. In this respect, we studied optical properties of palladium-coated core-shell AuNRs at the single particle level. The single particle measurement allowed us to eliminate the ensemble error and to gain more specific understanding on their optical properties. In this study, the core-shell nanoparticles were characterized by transmission electron microscopy (TEM), UV-Vis absorption spectrometry, dark-field (DF) microscopy, and differential interference contrast (DIC) microscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-8**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:08, 좌장: 하지원

Simultaneous determination of volatile organic compounds (VOCs) with a wide range of polarities in urine by headspace solid-phase microextraction (HS-SPME) coupled to gas chromatography-mass spectrometry

송한나 김종혁 이원용[1] 조성희*

한국화학연구원 화학분석센터 [1]연세대학교 화학과

Volatile organic compounds (VOCs), ubiquitous environmental pollutants, are the organic compounds that have a high vapor pressure at room temperature. VOCs have been classified as carcinogen to humans by the International Agency for Research on Cancer (IARC), because they can bind to DNA and cause cell mutations. Therefore, monitoring of VOCs in human urine is very important to evaluate correlation between exposure of VOCs and human disease. We developed the improved analytical method for the simultaneous determination of VOCs with a wide range of polarities in human urine samples by headspace solid-phase microextraction (HS-SPME) coupled to gas chromatography-mass spectrometry (GC-MS). In the improved method, bi-polar carboxen-polydimethylsiloxane (CAR/PDMS) fiber was used for the optimized extraction of 15 VOCs with a wide range of polarities including benzene, toluene, ethylbenzene, xylenes (BTEX), alkylbenzenes, cresols, and naphthalene in human urine samples and the parameters for SPME were optimized. Extracted VOCs from the human urine were effectively separated by GC using mid-polarity column (DB-35, 35% phenylmethylpolysiloxane) and monitored by mass spectrometry using selective ion monitoring (SIM) mode. Under the optimized method, the linearity of calibration curves was higher than 0.993. The limits of detection (LOD) at signal to noise (S/N) ratio of 3 were 0.3-0.6 ng/mL. The coefficients of variation were in the range of 0.1-9.7% for within-day variation and 0.2-14.2% for day-to-day variation, respectively. The present method was highly sensitive and simple for simultaneous determination of VOCs with a wide range of polarities in human urine and could be applied to monitoring and biomedical investigations to check exposure of VOCs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-9**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:11, 좌장: 하지원

Determination of Polycyclic Aromatic Hydrocarbons (PAHs) in Human Urine Samples by High-Resolution Gas Chromatography-Mass Spectrometry for Excretion Pattern Study

이선경 김종혁[1] 이상원 조성희[1,*]

고려대학교 화학과 [1]한국화학연구원 화학분석센터

Polycyclic aromatic hydrocarbons (PAHs), the organic compounds formed by at least two condensed aromatic rings, are ubiquitous environmental pollutants that are produced by incomplete combustion of organic materials. PAHs have been classified as carcinogen to humans by the International Agency for Research on Cancer (IARC), because they can bind to DNA, causing mutations. Therefore, the levels of PAHs in human urine samples can be used as an indicator for potential carcinogenesis and cell mutation. In this study, to investigate association between excretion patterns of 18 PAHs in human and carcinogenesis, the analytical method was developed for the measurement of carcinogenic PAHs in human urine using high-resolution gas chromatography-mass spectrometry (HR-GC-TOF/MS). Urine samples were extracted by an Oasis HLB extraction cartridge after enzymatic hydrolysis with β-glucuronidase, arylsulfatase, or β-glucuronidase/arylsulfatase cocktail. The 18 PAHs were separated using Agilent DB-5 MS capillary column (30 m x 0.25 mm, 0.25 μm) and monitored by time of flight (TOF) mass spectrometry with the selected ion-monitoring (SIM) mode. The linearity of this method was over 0.994. The limits of detection at signal to noise (S/N) ratio of 3 were 10 ~ 100 ng/L. The coefficients of variation were in the range of 0.2 -9.0% for within-day variation and 0.4-6.5% for day-to-day variation, respectively. The levels of PAHs in human urine and excretion pattern may play important role to understanding probable carcinogenesis induced by metabolism of PAHs, and the described methods could be used to evaluate and monitor exposure of PAHs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-10**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:14, 좌장: 하지원

Single Particle Study on the Optical Property of Pt-coated Core-Shell Gold Nanorods

김근완 하지원*

울산대학교 화학과

Various nanoparticles such as gold nanocubes, gold nanostars and gold nanorods (AuNRs) have been widely studied during past two decades. Recently, bimetallic core-shell nanoparticles have attracted great attention because of their unique optical properties resulted from localized surface plasmon resonance (LSPR) effect. Furthermore, bimetallic core-shell nanoparticles show unanticipated catalytic properties such as high catalytic activity, catalytic selectivity, and better resistance to deactivation. In this study, we investigated individual Pt-coated AuNRs under single particle spectroscopy without ensemble averaging. More specifically, far-field dark-field (DF) microscopy and differential interference contrast (DIC) microscopy were used to obtain optical images of Pt-coated AuNRs and characterize their optical properties at the single particle level.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-11**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:17, 좌장: 하지원

Spectroscopic and electrochemical studies of iodine substituted monoclinic $LiFeBO_3$ as a cathode material for Li-ion batteries

이한솔 이영일* 이형동

울산대학교 화학과

There are intensive research activities into alternative electrode materials for the next generation of Li-ion batteries, particularly for use in hybrid electric vehicles and grid scale battery. Monoclinic structured lithium metal borate, $LiMBO_3$ (M = Mn, Fe and Co) for cathode material of Li-ion battery have attracted great interest due to the lowest weight polyanion BO_3^{3-} which offers high theoretical capacity (220mAh/g), environmental friendliness, and high energy density with small volume change of 2%. However, lithium metal borates are considered to have intrinsically low ionic and electronic conductivity which is believed to be the cause of the poor electrochemical performance. Iodine substituted $LiM(BO_3)_{1-x}I_{3x}$ (M=Fe) have been proposed as alternatives to the conventional cathode material. $LiFe(BO_3)_{1-x}I_{3x}$ (x= 0.001, 0.002, 0.003) was synthesized by solid state reaction process. Among them, $LiFe(BO_3)_{1-x}I_{3x}$ (x=0.001) shows the best cycleability. It is characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) and electrochemical test. ^{7}Li MAS NMR was investigated to find lithium local structure of $LiFe(BO_3)_{1-x}I_{3x}$. ^{7}Li MAS NMR spectra of $LiFe(BO_3)_{1-x}I_{3x}$ (x= 0.001, 0.002, 0.003) shows a single isotropic peak with spinning sidebands.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-12**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 하지원

Customized home-built solid-state NMR probes for biological samples and electronic device

최성섭 정지호 김용애*

한국외국어대학교 화학과

The solid-state NMR has recently developed to investigate insoluble materials. It could be applied to a broad range of organic/inorganic nano-materials including polymers and bio-solids including pharmaceutical drugs and membrane proteins. Solid-state NMR spectroscopy is very valuable to study the structure and dynamics of membrane proteins even though most biological samples on lipid bilayers have high dielectric property due to containing large amounts of lipids, water and salts. We try to make the specific probe with high efficiency and durability for biological samples. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) 1H-15N solid-state NMR probe and a home-built 800 MHz narrow-bore (NB) 1H-15N solid-state NMR probe for these lossy membrane proteins.Li-ion battery and LCD panel have been grown up rapidly as a front-runner in technology-intensive industry. Their microstructural changes are the reason of battery efficiency drop and defective pixel. We will also present a home-built 500 MHz NB 19F-13C solid-state NMR probe with flat-square coil for analyzing LCD panel and 600 MHz NB 19F-7Li solid-state NMR probe with solenoidal coil for investigating Li-ion battery. These were the first application for the in-situ analysis of LCD panel and in-situ analysis of Li ion battery pack samples. These two probes provide high efficiency and good RF homogeneity.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL1.O-13**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 10:23, 좌장: 하지원

Strategies employed in the characteristics of antimicrobial peptides with enhanced activities derived from Lactophoricin

정지호 김지선 김용애*

한국외국어대학교 화학과

In recent years, spread of antibiotic resistance bacterial pathogens have been considerable interest in investigations of new class of antimicrobial molecules, antimicrobial peptides (AMPs). AMPs are usually relatively short positively charged polypeptides and exhibiting amphipathic character. Despite significant differences in their structures, all AMPs discovered share the ability to interact with cellular membranes, thereby disrupting membrane organization. Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, was currently utilized as the framework to design the novel analogs and study the effect of peptide hydrophobicity/hydrophilicity, amphipathicity on antimicrobial activities. LPcin analogs were designed and modified to enhance antibacterial activity using conservative sequence change. Three promising candidates were selected among LPcin analogs using bacterial killing and growth inhibition assays against Gram-negative and Gram-positive bacteria. We successfully overexpressed LPcin analogs in the form of fusion protein in Escherichia coli and purified them from the cell extracts with many biophysical techniques. In order to elucidate the structure-antibiotic activity relationships of the peptides, we studied the correlation between the modified conformation of LPcin analogs and their antimicrobial activity using various spectroscopic methods like MALDI-TOF MS and CD spectrometry, as well as 1D/2D solution NMR spectroscopy and 1D/2D solid-state NMR spectroscopy in membrane mimic environments. The structural calculations of LPcin analogs using Discovery Studio 2016 were also used to refine the orientational information of 3D structure and topology based on 2D SAMPI4 solid-state NMR spectra.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-14**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:26, 좌장: 하지원

Study of the electrochemical performance for nickel substituted olivine-monoclinic complexes as a cathode material for Li-ion batteries

이지원 이영일* 박재영 지민수

울산대학교 화학과

The olivine structured LiMPO$_4$ (M= Fe, Co, Ni) as an attractive cathode material for Li-ion batteries has been investigated due to low cost, eco-friendly, and structural stability. However, olivine materials have relatively poor electrochemical performance compared to other structure of cathode materials such as layered structure $LiCoO_2$, spinel structure $LiMn_2O_4$, and monoclinic structure $LiFeBO_3$. It is known that the mixing of olivine and monoclinic structured material is improved the specific capacity. Moreover, nickel substitution in metal site is suggested in this presentation to increase operate voltage and conductivity. The olivine-monoclinic complex materials have been synthesized by solid-state reaction using planetary mill. The morphology, compositions, and electrochemical performance of the synthesized sample were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), cycling test, galvanostatic charge-discharge measurement, etc.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-15**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:29, 좌장: 하지원

Quantitation of arsenic species in white rice and brown rice using LC-ICP-MS System

박미선 김관수*

동일시마즈(주) 지원본부

Rice is one of the agricultural products including a relatively significant amount of arsenic in which the ratio of inorganic arsenic is commonly known to be high. Codex Alimentarius Commission held in July 2014 decided to be 0.2 mg/kg over the maximum content of inorganic arsenic in polished rice. Arsenic species have each inherent poisonous property. The poisonous property of inorganic arsenic is known to be higher than that of organic arsenic. An LC-ICP-MS system which connects an inductively coupled plasma mass spectrometer (ICP-MS) in-line with a high-performance liquid chromatography (HPLC) system allows the high sensitive and high accuracy measurement of arsenic species. The quantitation of inorganic arsenic species [As(III) and As(V)] and dimethylarsinic acid in white rice and brown rice was accomplished by connecting the ICPMS-2030 in-line with a HPLC system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-16**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:32, 좌장: 하지원

피톤치드가 첨가된 PSA의 성능평가에 관한연구

김경석 전보현 서예지 김성호[*]

순천향대학교 화학과

피톤치드는 식물에 존재하는 향으로써 스트레스 완화작용, 항균작용 등이 알려져 있으며, 방향제, 천연 세제 등 여러 형태로 이용되고 있다. 본 연구에서 점착제 층에 피톤치드를 첨가하여, 패치를 제작하고, 피톤치드의 유효성능유지기간, 점착력, 유지력등을 측정하는 방법으로 그 성능을 평가하였다. GC-MS 를 이용한 정성분석, HPLC 를 이용하여 정량분석을 실시하였으며, Ball Tack, peel strength, 유지력등을 측정하여, 성능이 우수한 피톤치드 패치를 개발하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-17**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:35, 좌장: 하지원

라벤더 향이 첨가된 패치의 점착성능 평가

전진 유하나 문지연 김성호*

순천향대학교 화학과

최근 천연오일의 효능이 밝혀짐에 따라 다양한 형태의 향 이용 방법이 개발되고 있다.그 중 수명과 효능을 오래 지속시키는 방법의 하나로 패치가 이용되고 있다. 패치 제작시 PSA 에 라벤더 오일을 첨가한다. 본 연구는 패치의 PSA 에 첨가된 라벤더오일을 GC-MS 와 HPLC 를 이용하여 정성, 정량 분석하여 첨가된 라벤다의 유효 시간을 측정 하였으며, 향의 함량변화에 대한 초기점착력, 유지력 변화등을 측정하는 방법의 패치의 성능을 평가 하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-18**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:38, 좌장: 하지원

Hyperpolarized Silicon Nanoparticles as Biocompatible Contrast Agents for 29Si Magnetic Resonance Imaging

서형림 최익장 고혜지 공경현 박희정[1] 정회일[2] 이영복*

한양대학교 응용화학과 [1]한국기초과학지원연구원 서울서부센터 [2]한양대학교 화학과

Silicon-based nanoparticles have been attracting a lot of interest in the field of biomedical applications due to their biocompatibility and biodegradability in vivo, as well as their flexible surface chemistry. Here, we demonstrate two different synthetic approaches in order to yield various nano-sized silicon nanoparticles (Si NPs) ranging from 5 nm to 500 nm as hyperpolarized contrast agents for magnetic resonance imaging (MRI). i) The particles were synthesized by means of a chemical reduction of micelles formed by mixing silicon tetrachloride and alkyltrichlorosilane. ii) Magnesiothermic reduction of silica was also processed to produce Si NPs. The Si NPs have many great benefits to the hyperpolarized MR imaging. Since a core region of the crystalline Si NPs is mostly protected from a main relaxation source, such as paramagnetic centers existing at surface defect sites, the Si NPs show extremely long depolarization times (usually longer than 30 mins), resulting in high MR image contrast with minimum or no background signals. In addition, paramagnetic centers on the surface defect sites play a pivotal role in generating MR signal enhancement induced by dynamic nuclear polarization (DNP) mechanism, thereby not necessary to add external radical sources. In conclusion, these features and benefits convincingly suggest that the Si NPs can potentially be used as a biocompatible, targetable, and hyperpolarized MRI contrast agents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-19**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:41, 좌장: 하지원

Synthesis and characterization of Silicon/reduced Graphene oxide composite film as anode for lithium ion batteries

이상훈 김용재 손빛나 최진영 이호춘[1] 이창섭*

계명대학교 화학과 [1]DGIST 에너지시스템공학

Silicon (Si) has been used as one of the most attractive anode materials for lithium-ion batteries because of its large theoretical capacity, high safety, low cost and environmental benignity. However, Silicon-based anode material needs to overcome the structural change of the solid-electrolyte interphase due to the large volume change during cycling. To resolve these problems, we have synthesized Si/rGO composite using graphene with superior conductivity, large specific surface area and flexibility. The Graphene oxide(GO) solution was deposited on the copper foil for 10 min to form a GO layer. Then the Si-containing solution was deposited for 5 min to form a Si-doped layer. Finally, the multi-layered structure was obtained by depositing GO and Si-doped layers alternately. After heat treatment by thermal chemical vapor deposition(CVD), the resulted Si/rGO composite film on copper foil was obtained. The characteristics of Si/rGO composite were analyzed by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of Si/rGO as anodes of Li ion batteries were investigated using coin cell and battery tester.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL1.O-20**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 10:44, 좌장: 하지원

Synthesis and Electrochemical Performance of Transition metal-coated Carbon Nanofibers as Anode Materials for Lithium Secondary Batteries

최진영 현유라 황은정 박희구[1] 이창섭*

계명대학교 화학과 [1]계명대학교 화학시스템공학과

In this study, transition metal coated carbon nanofibers (CNFs) were synthesized and applied as anode materials of Li secondary batteries. The CNFs/Ni foam was put into the 0.01 M transition metal solutions after the CNFs were grown on Ni foam via chemical vapor deposition (CVD) method. The transition metal coated CNFs/Ni foam was dried in a dryer at 80 ℃. The morphologies, compositions, and crystal quality of transition metals/CNFs/Ni foam were characterized by SEM, EDS, XRD, and Raman spectroscopy. The electrochemical characteristics of transition metals/CNFs/Ni foam as anode of Li secondary batteries were investigated using three-electrode cell. The transition metals/ CNFs/Ni foam was directly employed as a working electrode without any binder, and lithium foil was used as the counter and reference electrodes. 1 M $LiClO_4$ was employed as electrolyte and dissolved in a mixture of propylene carbonate (PC) : ethylene carbonate (EC) in a 1:1 volume ratio. The galvanostatic charge/discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. In particular, synthesized transition metals/CNFs/Ni foam showed the highest retention rate (41%). The initial capacity (670 mAh/g) was reduced to 275 mAh/g after 30 cycles.

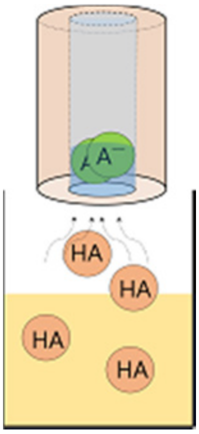
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-21**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:47, 좌장: 하지원

Headspace intube microextraction for capillary electrophoresis mass spectrometry for analysis of hydrophilic volatile molecules

권준엽 최윤정 정두수*

서울대학교 화학부

Capillary electrophoresis mass spectrometry (CE/MS) is appropriate analysis method for small amount of samples. However CE/MS lacks of online sample extraction method. We previously made headspace single drop microextraction (HS-SDME) for CE/MS. HS-SDME showed high enrichment factor (EF) and reproducibility. But HS-SDME required improvised outlet vial for drop formation which needs skillful handworks and risks electrospray needle conditions. Headspace intube microextraction (HS-ITME) uses no drops, only exposed area of acceptor in capillary section. HS-ITME shows lower EF than HS-SDME, but HS-ITME requires no improvised vial or modification to electrospray ionization area. We applied short chain fatty/organic acids and chlorophenols as examples. EF, comparing with normal CE/MS, showed 20~30 for 15 min extraction under room temperature. The HS-ITME is expected to increase effectiveness of CE/MS.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-22**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:50, 좌장: 하지원

Application of Ultra-high resolution 2-Omega FT-ICR MS for the Analysis of Complex Mixture

조은지 김성환*

경북대학교 화학과

It is important to understand the chemical compositions of complex mixture including crude oil. There are many studies on analyzing the chemical compositions of crude oil using ultrahigh-resolution mass spectrometry (UHR-MS). Analysis of crude oil using Fourier transform ion cyclotron mass spectrometry (FT-ICR MS) has a great advantage. In those application, resolution and mass accuracy plays a key role in accessing accurate chemical compositions. The resolution of FT-ICR MS is increased proportional to the measured frequency. A new technique called "2-Omega" has been recently developed. In the technique, two pairs of electrodes comprising FT-ICR MS detector cell are used for detection. Therefore, the measured resolution is supposed to be doubled compared to the old design where only one pair of electrodes is used for detection. In this study, ultrahigh resolution mass spectra of crude oil were obtained and presented. The obtained mass accuracy and resolution are presented. The resolution of 2-Omega FT-ICR MS spectra were well over one million. The data were also examined to check the existence of 1-Omega peaks because they can cause mis-interpretation. The data presented in this study clearly shows that 2-Omega FT-ICR MS can be very useful in the analysis of complex mixture such as crude oil. To the best of our knowledge, this is the first report on the application of 2-Omega FT-ICR MS to study crude oils.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL1.O-23**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:53, 좌장: 하지원

Energy Dependent Tandem Mass Spectrometry Analysis for Structural Identification of Polycyclic Aromatic Hydrocarbons

하지현 김성환*

경북대학교 화학과

PAH (Polycyclic Aromatic Hydrocarbon) compound are common molecules found in the environment as well as Crude Oil. Some PAH are significant pollution source in the human body or the environment. In addition, PAHs include several isomers. It is important to analyze PAH compounds including structural isomers. One of the most widely used methods for PAH compounds is Liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). However, only a few publications reporting high resolution MS/MS spectra of PAHs are currently available. In addition, further limited number of publication is available focused on energy dependent MS/MS spectra of PAHs. In this study, it is hypothesized that obtaining MS/MS spectra with different collision energies and comparing the energy dependent pattern can be a useful tool to distinguish PAH isomers. To test the hypothesis, MS/MS spectra of 50 PAH compounds were obtained at various collisional energy and fragmentation patterns of PAHs depending on collisional energy were compared. Our results show that PAH isomers could be successfully distinguished from their significantly different relative ion intensity in the spectra obtained with various collision energies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-1**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:00, 좌장: 하지원

Enantioseparation of acidic chiral compounds on a clarithromycin-zirconia hybrid monolith by capillary electrochromatography

김미연 박정학*

영남대학교 화학과

A weak anion exchanger chiral selector, clarithromycin-incorporated zirconia hybrid monolithic (CLA-ZHM) capillary column was prepared by sol-gel technology. A sol solution consisting of 5.5 mM of polyethylene glycol, 1 mM of water, 3 mM of acetic acid, 2 mM of formamide, and 0.04/0.96 ratio of CLA-TEOSPC/Zr-Bu resulted in a homogeneous monolith having well defined through-pores and tightly anchored to the capillary wall. The CLA-ZHM column was employed for capillary electrochromatographic enantioseparation of ten acidic chiral drugs in mobile phases consisting of acetonitrile (ACN), methanol (MeOH) and triethylamine (TEA)-acetic acid (AcOH) buffer. Effects of ACN/MeOH ratio, AcOH/TEA ratio and their concentrations, and applied voltage on chiral separation were investigated. Baseline resolutions of all the compounds were achieved with a mobile phase of 70:30 (v/v) ACN/MeOH containing 255 mM AcOH and 17.4 mM TEA under the applied voltage of –10 kV at 25 °C.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-2**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:03, 좌장: 하지원

In situ Monitoring of Thermal Crosslinking Reaction and Residual Vinyl Group of Re-adhesive Organosilicon by VT-NMR

설혜원 이태희[1] 이태곤[1] 김정권[*] 김종혁[1,*]

충남대학교 화학과 [1]한국화학연구원 화학분석센터

The re-adhesive property of organosilicon is dependent on the residual vinyl group after the crosslinking reaction of hydrosilylation between vinyl group(Si-V, main chain) and hydrosilyl group(Si-H, crosslinker). When the vinyl group remains, we cannot expect good re-adhesive property because of adhesion over time. In this study, the end-point of crosslinking reactions was determined by variable temperature nuclear magnetic resonance(VT-NMR) spectroscopy. The relationship between adhesion and the residual vinyl group was confirmed by monitoring the crosslinking reaction. Our experiments were done with organosilicon mixture of main chain and crosslinker which has the end- or side-chain vinyl group and hydrosilyl group. Temperature was raised from 298 K to 373 K at a rate of 1.25 K/min and the spectra were recorded for a minute at each 5 K. The end-points of crosslinking reaction were determined by the loss of vinyl group signals and the appearance of crosslinking network($Si-CH_2-CH_2-Si$) signal in distortionless enhanced by polarization transfer(DEPT) spectrum. In case of the most vinyl-terminated poly-dimethylsiloxane, vinyl group signal was disappeared below 373 K. When a vinyl group is positioned beside backbone(vinyl-methylsiloxane), however, it still remained until 373 K. Additionally, we also investigated samples from a supplier and compared the results with our initial work. The adhesive remnant indexes(ARI) were almost the same when the vinyl group signal disappeared, while it changed when the vinyl group signal remained.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-3**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:06, 좌장: 하지원

Characterization of the Weathered Oil and Soil Extract Originated from Crude Oil Spill Site by Paper Spray Ionization Mass Spectrometry

김동휘 차상원[1] 김성환*

경북대학교 화학과 [1]한국외국어대학교 화학과

Oil spills have drawn the attentions of the researchers for their potential threats as well as direct influences to the environment and human beings.Once oil is spilled that goes through various reactions such as biodegradation and photodegradation, so that chemical compositions of the spilled oil are changed by weathering process. Besides, those reactions produce various toxic materials.Petroleomics using ultra-high resolution mass spectrometer(UHR-MS) has emerged as a powerful technique for analyzing petroleum and its product. ESI, APPI, and APCI are the most common ionization techniques for characterization of petroleum products. Even though those are very useful techniques, there are some limitations associated with solvent selection, sample amount and clogging problem. Therefore, application of new ionization technique can be beneficial.Recently developed paper spray ionization (PSI) is fast and convenient ionization method for the direct analysis of complex mixtures with minimum sample preparation. In addition, ionization and subsequent MS analysis can be done with small amount of sample when compared with aforementioned ionization techniques.In this study, weathered oil and soil extract from Hebei Spirit oil spill site in Taean have been characterized by paper spray ionization mass spectrometry.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-4**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:09, 좌장: 하지원

Investigating Photo-oxygenation tendency of Compounds with OLED Basic Structures by PSI Orbitrap and MALDI-TOF MS and Theoretical Calculation

박은영* 하지현 김성환

경북대학교 화학과

Organic light editting diode (OLED) utilize organic compounds that emit light after receiving electrical signals through electrical currents. The OLED is often commercially used to make displays for computers, smart-phones and various other electronic devices. However, when the components of OLED are photo-oxidized, impurities are created and the color of the display is changed. Compounds used for OLED typically have anthracene as basic structure. There are many compounds substituted at 9, 10 positions of anthracene. However, the effect of side chain on the oxidation rate has not been investigated yet. Therefore, in this study, samples having anthracene as core structure and 9 and/or 10 positions substituted with phenyl, methyl, or naphthyl groups were studied. The samples were oxidized with UV lamp under flow of oxygen gas. The observed rate of oxidation was different for each functional group. The Paper Spray Ionization (PSI) and Laser Desorption Ionization (LDI) mass spectrometry were used to analyze the oxidized samples. Theoretical calculations have been performed to explain the observed data.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-5**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:12, 좌장: 하지원

Study on Molecular Dynamics (MD) Simulations for Long Alkyl Chain Aromatic Compounds by using Ion Mobility Mass Spectrometry

임동완 김성환*

경북대학교 화학과

Travelling Wave Ion Mobility Spectrometry Mass-Mass Spectrometry (TWIMS-MS) is technique used to study shape and conformation of small molecules and proteins in gaseous ions. Furthermore, the analysis for Polycyclic Aromatic Hydrocarbons (PAHs) compounds in Crude oil is still one of important modern research issues. Especially, a detailed structural characterization of the involved PAHs compounds with alkyl chains is one of the remaining challenges in petroleomics. Our previous study (Ahmed, A. et al., Anal.Chem. 86, 3300-3306, 2014) has already shown the advantage of combining two well established MS techniques with theoretical Collisional Cross Section (tCCS) calculations to increase the amount of information gained as well as to determine the molecular structures of aromatic compounds. However, the result of previous study was limited to determine non-alkylated or short alkyl chains aromatic compounds. In this study, we employed temperature dependent molecular dynamic (MD) simulation to improve the CCS calculation accuracy, especially for long alkyl chain containing aromatic compounds. The Molecular Dynamic Simulation results of all the compounds correlates better with experimental results at high temperatures.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-6**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:15, 좌장: 하지원

Non-invasive detection of inner layer materials in turbid media using Deep Raman Spectroscopy

조영호 지민호 배창현 박찬량[1,*] 김형민[*]

국민대학교 생명나노화학과 [1]국민대학교 화학과

One of the most goals of the analytical technique in industrial fields is the provision of chemically fingerprinting, non-invasive method for monitoring the raw material composition in opacity media such as poly-ethylene case. Recently, the deep-Raman techniques play an important role in non-invasive and chemically specific analysis methods such as spatially-offset Raman spectroscopy (SORS). In this study, we demonstrate deep layer materials in turbid media without unpackaged using non-invasive deep Raman technique such as spatially offset Raman spectroscopy (SORS), line illumination spatially offset Raman spectroscopy (L-SORS) and line illumination one shot imaging techniques. Furthermore, the deep Raman methods are adopted to confirm their possibility for raw materials monitoring without unpackaged in pharmaceutical and industrial fields.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-7**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:18, 좌장: 하지원

Non-destructive Analysis of Traditional Korean Pigment Using Resonance Raman Scattering

송시원 박수빈 유익한 김규호[1,*] 박찬량[2,*] 김형민[*]

국민대학교 생명나노화학과 [1]공주대학교 문화재보존과학과 [2]국민대학교 화학과

Raman spectroscopy is the powerful spectroscopic tool that non-destructive in investigation of chemical compounds of materials. The Raman spectroscopy as a non-destructive methodology is demonstrated of published literatures [1]. It has not only non-destructive analysis but also a variety of advantages. It measures molecular vibration mode from scattering light according to lasers. Therefore it detects to the chemical composition, bonding, and structure of the sample material [2]. Furthermore, the Raman spectroscopy has benefit such as in situ monitoring and portability. These characteristics provide sensitive measurement to analysis at art and cultural properties because of the Raman spectroscopy do not damage at sample that have substantially historic worth and also provide a chemically fingerprint about the identification of materials. However, pigments had variable colors interrupt to measure Raman signal because of its radiating fluorescence. Therefore, we study identification of traditional Korean pigments using variable lasers. These are important to avoid fluorescence and take enhanced Raman signal from the resonance Raman scattering (RSR) effect that increases scattering efficiency because of that is related region of electronic state [3]. Resonance Raman measurement was performed a microscope (Olympus Bx73) that coupled to a spectrometer (Andor Shamrock 303i) with charge coupled devices (Andor iDus 420) using by 488 nm Ar-ion, 532 nm diode, and 632.8 nm He-Ne lasers. The pigment is used lumber painted Korean traditional pigment such as painted Sungnyemun Gate. In conclusion, we study using the resonance Raman methodology for analysis of pigments that have color be of help chemical identification and make database. It be of help for preservation and restoration Korean cultural properties.1.G. Burrafato, M. Calabrese, A. Cosentino, A. M. Gueli, S. O. Troja, and A. Zuccarello, ColoRaman project:Raman and fluorescence spectroscopy of oil, tempera and fresco paint pigment, Journal of Raman Spectroscopy 35, 879-886 (2004).2.G. D. Smith, and R. J. H. Clark, Raman microscopy in archaeological

science, Journal of Archaeological Science 31, 1137-1160 (2004).3.D. Gill, R. G. Kilponen, and L. Rimai, Resonance Raman Scattering of Laser Radiation by Vibrational Modes of Carotenoid Pigment Molecules in Intact Plant Tissues, Nature 227, 743-744 (1970).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-8**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:21, 좌장: 하지원

Carbomylated azithromycin-incorporated zirconia hybrid monolith for enantioseparation of acidic drugs using non-aqueous capillary electrochromatography

dixitshuchi 박정학*

영남대학교 화학과

Carbomylated derivatives of two antibiotics, namely, clindamycin phosphate (CLIP) and erythromycin (ERY) were successfully employed as co-precursors, in combination of zirconium tetrabutoxide as a precursor, to prepare chiral organic-zirconia hybrid monoliths (i.e., CLIP-ZHMs and ERY-ZHMs, respectively) via a single-step in-situ sol-gel approach in our previous works [1,2]. Their superiority over chiral organic-zirconia/silica monoliths, prepared by post-modification approach, in terms of better enantioresolution and enhanced stability inspired us to prepare ZHMs based on an another antibiotic, azithromycin (i.e., AZI-ZHMs). Monolithic columns were employed for capillary electrochromatographic enantioseparation of acidic chiral drugs in mobile phases consisting of acetonitrile (ACN) and methanol (MeOH) as organic modifiers and, acetic acid (AcOH) and triethylamine (TEA) as electrolytes. The effects of composition of mobile phase and applied voltage on chiral separation were investigated by using ketoprofen as a representative analyte. Baseline resolutions (i.e., Rs >1.5) were obtained for six acidic drugs (namely, ketoprofen, suprofen, carprofen, flurbriprofen, ibuprofen and warfarin) using a mobile phase consisting of 70/30 (v/v) ACN/MeOH with 240 mM AcOH and 20 mM TEA. The relative standard deviations for resolution values regarding column to column and batch to batch repeatability were less than 2.5% (for n=3) under optimized conditions indicating satisfactory stability of columns and reproducibility of column preparation process. [1]Dixit, S., Park, J. H., J. Chromatogr. A 2015, 1416, 129-136.[2]Tran, L. N., Dixit, S., Park, J. H., J. Chromatogr. A 2014, 1356, 289-293.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-9**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:24, 좌장: 하지원

Laser Desorption/Ionization Mass Spectrometry Analysis of Boron Nitride

배광태 조수경[1,*] 유해욱[2]

국방과학연구소 4본부 2부 [1]국방과학연구소 4본부-2부 [2]국방과학연구소 4본부2부

Laser desorption/ionization (LDI) mass spectrometry is one of useful analytical instruments in identifying high energy species from various precursors. We have been investigating nitrogen-rich high energy species starting from azoles, azides, and other compounds generating nitrogen-rich species [1]. Boron nitride is one of promising precurors which may generate highly energetic nitrogen-rich species. In addition, boron species are also known to hive high energies. We performed LDI experiments on solid boron nitride and analyzed with time-of-flight mass spectrometry (TOF MS). Various ionic BxNx clusters of B+, B2+, BN+, N2+, B3+, B2N+, N4+, B3N2+, B4N3+ were identified in positive MS mode. Further, we will present energy diagrams and reaction mechanisms of these highly energetic species.[1] Cho, S.G.; Bae, K.T.; Goh, E.M. Bae, S.W.; Shin, I.-S. Bull Korean Chem. Soc, 2016, 37, 99-102.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-10**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:27, 좌장: 하지원

Relative Quantitation of N-linked Glycans in Rice using Metabolic Isotope Labeling by Mass Spectrometry

서현경 김진화 임재민*

창원대학교 화학과

Glycosylation is one of the most common post-translational modifications in biological system. Glycan play significant roles for a wide range of biological processes regulating such as cell-cell interactions, cell division and adhesion, cellular recognition, immune response, and protein stability. For the purpose of understanding the biological relevance of glycans, many mass spectrometry based methods have been developed for the relative quantitation of glycan.Herein, we describe a new *in vivo* labeling method either normal or heavy glucose to tag glycans from rice culture. Isotopic glucose enters the glucose metabolic pathway, which in turn produces nucleotide sugars precursors that are subsequently used for all glycan biosynthesis.Thus, each of sugars in glycan occur a mass shift as much as 1 Da. For glycan containing five sugars, occurs a mass shift of as much as 5 Da. A method for relative quantitation of glycans by ratio of normal glucose labeled glycan and heavy glucose labeled glycan.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-11**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:30, 좌장: 하지원

Simultaneous Determination of Estrogens in Environmental Aqueous Samples by Dispersive Liquid–Liquid Microextraction and HPLC/UV-Vis

문연주 조현우[1] 명승운*

경기대학교 화학과 [1]경기대학교 자연과학화학과

The objective of this study was to optimize dispersive liquid–liquid microextraction (DLLME) parameters for the simultaneous sample preparation of five steroidal estrogens (estrone (E1), 17α-estradiol (αE2), 17β-estradiol (E2), 17 α-ethinylestradiol (EE2), and estriol (E3)) from environmental aqueous samples. Estrogens were extracted and concentrated simultaneously an aqueous sample using dispersive and extraction solvents, and chromatographic separation and quantitative analysis were performed by an HPLC/UV-Vis system. It was evaluated optimum parameters for the effects of the combination of dispersion and extraction solvent, ionic strength, and sample pH. The optimized results gave increased enrichment factors (EF = 28.4–69.4). From the established extraction condition, the limits of detection and quantification in the spiked samples were in the concentration ranges 0.03–0.07 mg/L and 0.10–0.23 mg/L, respectively. The method gave good linear calibration curves with correlation coefficients (r_2) of 0.9990–0.9995 in the 0.10-8.00 mg/L. The relative recoveries and standard deviation in the calibration ranges were 99.1–116.6% and 0.6–4.2% (RSD), respectively. The proposed method, which is fast, simple, inexpensive, and environmental friendly, can be applied to the effective and simultaneous analysis of five steroidal estrogens from environmental aquatic samples.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-12**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:33, 좌장: 하지원

Using EME for Determination of NSAIDs by HPLC-UV

김진문 조현우[1] 명승운*

경기대학교 화학과 [1]경기대학교 자연과학화학과

The electromembrane extraction(EME) is one of the liquid phase microextraction(LPME) which can extract and concentrate the analyte from aqueous matrices such as urine and plasma effectively. This method was applied to analysis of six Non-steroidal anti-inflammatory drugs(NSAIDs) in aqueous samples. The parameters such as pH of acceptor and sample, stirring speed, voltage, support liquid membrane(SLM), and extraction time were optimized. Simultaneous chromatographic separation of six NSAIDs by HPLC-UV/Vis system was achieved on an Eclipse XDB-C18 (4.6 mm i.d. × 150 mm length, 5 ㎛ particle size) column using gradient elution with 0.1 % formic acid and methanol. 0.1 % formic acid and methanol start to 20:80 and after 7minutes, compositon and flow rate are changed to 15:85, finally, back to the first condition after 5minutes. After the extraction, 5 ㎕ of extract was directly injected into the HPLC-UV system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-13**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:36, 좌장: 하지원

FT-IR microscopic study of human hairs in various pH solution

김혜영 권오선 유수련[1] 신관우[2,*]

서강대학교 화학과 [1]서강대학교 화학과,바이오계면연구소 [2]서강대학교 화학과 및 바이오융합과정

In this research, natural and intact hair is used and experiments are performed within pH range from 1 to 12. Given that nitrogen oxide is the major cause of acid rain, nitric acid was used for making acidic solution and for the basic one, normal potassium hydroxide was used. In each pH, cross-section images and IR spectrums are obtained with FT-IR microspectroscopy. Since a hair fiber can be divided into outer layer(cuticle) and inner part(cortex), comparisons between these two parts are also made in each section. From the controlled experiments, we will present how the human hairs can be affected and the detailed analysis of each protein component in various pH condition will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-14**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:39, 좌장: 하지원

Headspace in-tube microextraction of dichlorophenols using a commercial capillary electrophoresis instrument

최윤정 정두수*

서울대학교 화학부

Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are commonly employed for headspace (HS) extraction, which is useful for the concentration of volatile materials in a complex matrix. Among LPME methods, single drop microextraction (SDME) is widely used for HS extraction to be off-line coupled with GC and LC. By forming a single acceptor drop at the tip of a capillary using a commercial capillary electrophoresis (CE) instrument, we showed that SDME can be easily in-lined coupled with CE to achieve high sample enrichments in a short time. However, it is difficult to hang a drop of very small volume to a separation capillary in the HS stably for long extraction. Recently this problem was solved by in-tube microextraction (ITME) using the liquid plug inside the capillary as an acceptor phase without hanging a drop. HS-ITME-CE was performed to enrich dichlorophenol in an aqueous solution. To promote the evaporation of the acidic dichlorophenols into the HS as neutral forms, the donor was acidified by adding HCl. To promote back extraction from the HS, a short acceptor plug of 400 mM borate buffer of pH 9.3 was used. The subsequent CE was carried out using a run buffer of 240 mM borate buffer of pH 9.2. With a 15-min extraction at 80°C, dichlorophenols were enriched about 300 times.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-15**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:42, 좌장: 하지원

Automated liquid extraction surface analysis in-line coupled with sweeping for rapid and direct analysis of a solid surface sample

이호균 최윤정 정두수*

서울대학교 화학부

High performance separation and many other advantages such as a small volume sample requirement of capillary electrophoresis (CE) come from the fact of using a narrow-bore fused silica as a separation column. However, the small dimension of the detection path length causes poor detection sensitivity. To overcome this, sample preconcentration technique is needed. There were many preconcentration methods coupled with CE, but almost used liquid sample or homogenized solid bulk sample. Liquid extraction surface analysis (LESA) is a direct surface-sampling technique avoiding the dilution from sample pretreatment procedures including homogenization of a bulk sample. LESA was in-line coupled with homemade CE-laser induced fluorescence (LIF), but homemade CE was operated manually and sample was injected by gravity, so whole extraction procedure needed ~20 minutes. In this study, commercial CE instrument was used for rapid and automatic LESA, and extraction only took ~2 minutes. For separation neutral pesticides efficiently, we use sweeping for detect choloorantranili, kresoxim-methyl and paraclostrobin. The sensitivity was improved by sweeping compare with common micellar electrokinetic chromatography method.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-16**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:45, 좌장: 하지원

Three-phase direct immersion in-tube microextraction coupled with capillary electrophoresis

최지은 정두수*

서울대학교 화학부

Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are widely used for sample enrichment and cleanup prior to an instrumental analysis. Compared to simply applicable SPME, LPME requires more manual maneuvers. In order to overcome such shortcomings of LPME, we developed in-tube microextraction (ITME). ITME uses a liquid plug inside a capillary as an acceptor phase and thus can be in-line coupled with capillary electrophoresis (CE) with ease. Since the acceptor phase is well protected inside the capillary, ITME can be carried out under severe extraction conditions. Moreover, given that the extraction and injection processes take place simultaneously, the extraction speed and efficiency are very high. Recently we have demonstrated headspace ITME by placing a separation capillary filled with an acceptor plug in the headspace above a sample solution using a commercial CE instrument. Here, we present 3-phase direct immersion ITME coupled with CE. By immersing the separation capillary containing a basic acceptor plug and a thin organic plug into an acidic sample solution, weakly acidic analytes in the neutral form are partitioned into the organic plug, and then back-extracted into the basic acceptor plug, followed by CE. With a 3-min extraction, Ketoprofen, Ibuprofen and Naproxen were enriched 975, 1100, and 1110 times, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-17**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:48, 좌장: 하지원

SERS-based Wash-free Magnetic Immunoassay Using Sequential Droplet Merging and Splitting

최남현 고주희[1] 주재범[2,*]

한양대학교 바이오나노공학과 [1]한양대학교 나노센서연구소 [2]한양대학교 생명나노공학과

The combination of surface-enhanced Raman scattering (SERS) with microfluidic devices provides an ideal mechanism for achieving rapid, sensitive and reproducible detection of specific biomarkers in solution. An additional benefit of such platform is the use of minimal sample volumes and low analyte concentrations. We recently reported a SERS-based wash-free magnetic immunoassay technique using magnet-embedded droplet microfluidics. In this platform, the assay could be performed without any washing process by separating immunocomplexes from the supernatant solution using a magnetic separation. Nonetheless, this methodology still limited in assay because the channel structure for reagents injection and mixing is unified in a channel. To resolve this problem, a new class of microdroplet-merging device was designed and fabricated for sequential immunoassay. This device is composed of five distinct compartments such as droplets merging, separating immunocomplexes from supernatant solution, isolating magnetic immunocomplex droplets, and collecting unbound SERS probe droplets for detection. Herein, we report a novel SERS-based wash-free immunoassay device composed of compartments for mixing, merging, splitting and detection.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-18**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:51, 좌장: 하지원

Novel Strategy for Quality Assessment of Glycosylation on a Biotherapeutic Glycoprotein by Intact Protein Analysis

김운용 오명진[1] 서영숙[2] 문한태[2] 안현주[2,*]

충남대학교 AGRS [1]충남대학교 분석과학대학원 [2]충남대학교 분석과학기술대학원

Protein glycosylation plays an important role in determining in vivo bioactivity, stability, solubility, and metabolic fate of biotherapeutics. Thus, detailed glycomic analyses are necessary complement to ensure quality, safety, and potency of therapeutic glycoproteins during production process. Current methods such as bottom-up and middle-down approaches employing LC-MS and LC-MS/MS for the glycomic characterization of biotherapeutics provide valuable information regarding glycan structure, isomers, and micro-heterogeneity. However, these methods significantly demand massive time and efforts from sample preparation to data interpretation. For these reasons, glycan or glycopeptide based approach is not suitable for real-time quality control in manufacturing processes. This study aims to develop novel analytical tool for real time determination of glycosylation site-occupancy with micro-heterogeneity using intact protein analysis (native mass spectrometry) without any additional sample preparation steps which can provide comprehensive glycosylation information.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-19**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:54, 좌장: 하지원

A Novel SERS-based Lateral Flow Assay Sensor for Rapid and Sensitive Detection of Autoantibody Against Citrullinated Peptide

전향아 이상엽[1] 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Rapid, user-friendly and versatile lateral flow (LF) strips have been extensively used for point-of-care (POC) and site-of-care (SOC) diagnostics. However, they have major limitations in terms of detection sensitivity and limited quantification capability. To resolve these problems, we recently developed a novel surface-enhanced Raman scattering (SERS)-based LF assay sensor for the quantitative analysis of a specific biomarker [1,2]. To assess the potential utility of SERS-based LF sensor in rheumatoid arthritis (RA) diagnosis, we extended the use of SERS-based LF assay platform to clinical samples of RA patients. In the first part of this work, the SERS-based LF assay for autoantibody against citrullinated peptide (anti-CCP) spiked in human serum was performed. For this purpose, CCP-immobilized LF strips and human IgG-conjugated SERS nano tags were prepared. Then the SERS signal of immunocomplexes on the test line was measured. Second, the SERS-based LF assay sensor was applied for real RA patient human sera collected by Hanyang University Hospital for Rheumatic Diseases. The clinical samples were divided into anti-CCP positive and anti-CCP negative groups according to their assay results by a commercially available ELISA kit. Next, the SERS-based LF assay results were compared to those measured by the commercially available ELISA kit. Statistical analyses were performed to evaluate the correlation between the ELISA and SERS-based LF assay results for both anti-CCP positive and negative patient groups.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-20**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:57, 좌장: 하지원

Salivary Glycomic Approach for the Distinction of Human Constitutions

문한태 윤나영 김범진 안현주*

충남대학교 분석과학기술대학원

Unlike western medicine, oriental medicine has the constitutional diagnostics to determine individual health status. The accurate diagnosis of constitution is very important because therapy can be differed from patient’s constitution. Saliva, readily accessible and noninvasive fluid, contains mucins, which are heavily glycosylated proteins. Changes of glycosylation reflect health status because glycosylation is highly sensitive to the biochemical environment. In this study, we aim to conduct MS-based salivary glycomic approach to identify potential glycan signature for constitution classification. Saliva was collected from 9 normal people; 7 pancreotonia, 1 pulmotonia and 1 colonotonia. Initially, the saliva was filtered by 10K MWCO spin column to remove impurities. N-glycans were enzymatically released by PNGase F and purified by C18 SPE. Finally, the N-glycans were eluted by PGC SPE. For overall N-glycan profiling, both MALDI-TOF MS and nano-LC/Q-TOF MS were used to provide independent orthogonal analysis. Approximately 150 compositions of N-glycan were profiled and they were compared to identify the difference of glycans depending on presence (frequency), quantitation, composition, and structure. In constitution distinction, bi- and tri-antennary fucosylated N-glycans are high in abundance in pulmotonia and colonotonia while sialylated N-glycans are high in abundance in pancreotonia. MS-based salivary glycomic approach can be used as a discrimination system for the human constitution classification.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-21**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 하지원

Highly Sensitive Detection of Estradiol Using SERS-based Competitive Immunoassay for the Diagnosis of Precocious Puberty

WANGRUI 전향아 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Estradiol (E2) is a biologically active sex steroid hormone that serves as important diagnostic marker in serum of premenopausal and postmenopausal women and in men. Particularly, the serum E2 concentration is very low (< 10 pg/mL) in prepubertal girls. In the past decades, several technologies, including high performance liquid chromatography-mass spectrometry (HPLC-MS), gas chromatography-mass spectrometry (GC-MS) and immunoassays have been developed for the measurement of E2. Unfortunately, current clinical detection methods are insufficient for accurate assessment of E2 at low concentrations (< 10 pg/mL). Thus, there is an urgent need for new technologies with efficient and sensitive detection of E2 for use in routine clinical diagnostics. In this study, we introduce a new E2 assay technique using a surface-enhanced Raman scattering (SERS)-based detection method. The SERS-based assay was performed with 30 blood samples to assess its clinical feasibility, and the limit of detection of E2 using the novel SERS-based assay described in this study was 0.65 pg/mL. Furthermore, this method showed a good correlation compared with the commercially available chemiluminescent microparticle immunoassay (CMIA) kit. Thus, the proposed SERS-based assay has a strong potential to be a valuable tool in the early diagnosis of precocious puberty due to its excellent analytical sensitivity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-22**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:03, 좌장: 하지원

Simultaneous Detection of Dual Prostate Cancer Markers in Blood Serum Using SERS-Based Immunoassay

CHENGZIYI 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Prostate-specific antigen (PSA) is a 30-kDa serine protease. PSA in blood exists in dual forms; one is a free form and the other is a complexed form with the protease inhibitors a1-antichymotrypsin (ACT). Total PSA is a combination of both free and PSA/ACT complexed forms. Previous reports show that the clinical accuracy of PSA biomarkers can be improved by measuring the ratio between free-PSA and PSA-ACT in serum. In this work, we developed a novel SERS-based immunoassay technique for the simultaneous detection of both PSA/ACT and free-PSA biomarkers in serum. For this purpose, total-PSA antibody-conjugated magnetic beads and two different types of antibody-conjugated SERS nano-tags (MGITC labeled GNP conjugated with free-PSA monoclonal antibody (mAb) and XRITC labeled GNP conjugated with PSA/ACT mAb) were prepared. The assay was performed by the following procedure. First, total PSA antibodies were immobilized on the surface of a carboxyl-modified magnetic bead. Second, different ratios of PSA/ACT and free-PSA mixtures were prepared and added to the antibody-conjugated magnetic bead solution. Third, two different types of SERS nano-tags were added to the solution. Finally, the duplex sandwich immunocomplexes were isolated by a magnetic bar, and then the SERS signals of SERS nano-tags were measured and analyzed. This assay platform will be useful for the early diagnosis of prostate cancer patients.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-23**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:06, 좌장: 하지원

Nano-Pillar Array Chip for the Rapid and Sensitive Detection of Food Poisoning Bacteria

고주희 박성규[1] 이상엽[2] 주재범[2,*]

한양대학교 나노센서연구소 [1]재료연구소 표면기술연구본부 [2]한양대학교 생명나노공학과

Rapid and sensitive identification of pathogenic bacteria is a key factor for the early diagnosis of infectious disease. Serological culturing-based assays are extensively used for the identification of bacteria but it takes a long time due to their culturing process. Polymerase chain reaction (PCR) is another analytical tool for detecting bacteria. However, PCR also needs an amplification of target genes using thermo-cycling steps because the concentration of target gene sequence is relatively lower than that of unrelated gene sequences. In many cases, amplification process causes false-positive signals and wrong identification. To resolve these problems, we developed a novel amplification-free SERS imaging sensor for the rapid and sensitive detection of Salmonella typhimurium bacteria. This technique does not require any cell culture or DNA amplification processes due to its highly sensitive detection capability. For this purpose, we fabricated antibody-conjugated SERS nano tags and three-dimensional nanopillar-pattered SERS substrates. The analytical strategy involves 3 steps; (1) immobilization of capture antibodies on nano-pillar substrate, (2) capturing of bacteria using specific interaction between antibodies and bacteria, and (3) labelling of bacteria with SERS nano tags and their SERS imaging detection. This SERS-based imaging sensor allows the limit of detection (LOD) of Salmonella typhimurium bacteria as low as 4,000 CFU/mL without any sample enrichment process. This SERS-based imaging technique is expected to be a potentially useful tool for the rapid and sensitive detection of pathogenic bacteria.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-24**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:09, 좌장: 하지원

Application of Hansen solubility parameter to optimize extraction solvents of sample preparation methods

육한나 이민지 이성광*

한남대학교 화학과

Solubility parameter (SP) is an important physical and chemical properties for selecting a proper solvent. Both the total solubility parameter and its constituent partial solubility parameters(Hansen solubility parameters) are widely used for the selection of appropriate solvents for given solutes. The use of the solubility parameter for the selection of solvents is based on the well-known rule of chemistry: “like dissolves like.” Thus, if the intermolecular forces between the molecules of the solvent and between the molecules of a solute are of a similar strength, the solvent is usually a good solvent for this solute. In this study, we investigated the relation between solubility parameter of extraction solvent and that of analytes for sample preparation process such as solid phase extraction(SPE) and liquid-liquid extraction(LLE). The recoveries in a given system have been correlated by the difference between solubility parameter of solvents and that of analytes. This study will help to select optimum solvent for sample preparation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-25**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:12, 좌장: 하지원

QSPR studies for predicting the cloud point of nonionic surfactants

조승현 이민지 이성광*

한남대학교 화학과

Cloud point(CP) is the temperature above which aqueous solutions of non-ionic and zwitterionic surfactants become turbid. Cloud Point Extraction(CPE) is a separation and preconcentration procedure that has been extensively applied for trace metal and organic compound determination in agreement with the ‘‘green chemistry’’ principles compared to those extractions that use organic solvents. Considering the complexity of synthesis and CP measurement for nonionic surfactants, the optimization of CP determination is relatively tedious and time consuming. Thus, the computational approach becomes an ideal alternative for analyzing, interpreting, and predicting the properties of unknown molecules. This study aimed to predict cloud point of nonionic by using a quantitative structure-property relationship(QSPR) method. The data set of cloud point were collected from a series of 85 nonionic surfactants. The molecular descriptors in models were calculated by PreADMET program and dataset was divided into training and test set by using KNIME. The forward selection and bootstrap sampling method were applied to determine the optimum descriptor of the multiple linear regression(MLR) in RapidMiner. The performance of each model were compared with R^2 , RMSE(root mean square error), and MAE(mean absolute error) for training and test set. It was possible to know the applicable range of the prediction model by applicability domain(AD) of the results of each model. Y-scrambling was performed to confirm chance correlation of the model.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-26**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:15, 좌장: 하지원

Study on stability of lipid vesicle using asymmetrical flow field-flow fractionation (AsFlFFF) and dynamic light scattering (DLS)

김민욱 **최재영 한수정 Lars Nilsson[1] 이승호***

한남대학교 화학과 [1]Lund University

Vesicles are of microscopic structure and composition that enclose a volume with a molecularly thin membrane. Generally the membrane is a self-directed assembly of amphiphilic molecules with a dual hydrophilic-hydrophobic nature, and is a spherical shell composed of lipid bilayer that encapsulate an aqueous space. Vesicles have been used as nano-scale containers for drugs, model membranes and other substances in pharmaceutical and cosmetic industries. Generally the stability of vesicles is closely related with their size and size distribution. When vesicles are used for drug delivery, the stability, and thus their life-time is directly associated with the medicinal effects. Thus size characterization of vesicles is necessary for understanding of the vesicle stability. Various techniques including electronic microscopy (EM), nuclear magnetic resonance (NMR), dynamic light scattering (DLS) and nanoparticle tracking analysis (NTA) have been used for size analysis of nano-sized particulates. DLS is simple to use, and has been widely used for analysis of particle size and its distribution. The application of DLS is however rather limited when dealing with samples of complex mixtures or of broad size distributions. Field-flow fractionation (FFF) has been employed for size-based separation and size-characterization of particles having broad size distributions from a few nm up to about 100 μm. Asymmetrical flow field-flow fractionation (AsFlFFF), one of members of FFF family, is particularly useful for characterization of aqueous colloidal particles.In this study, nano-sized vesicles were prepared by extrusion with the lipid concentration varied from 0.5 to 1.5%, and then were analyzed by AsFlFFF for determination of the size distribution, the stability (and life-time) and the osmotic pressure. It was found that the stability of vesicle increases as the lipid concentration increases. It was also observed that the vesicle stability is affected by the osmotic pressure.

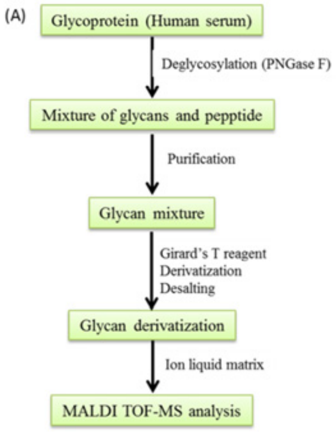
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-27**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:18, 좌장: 하지원

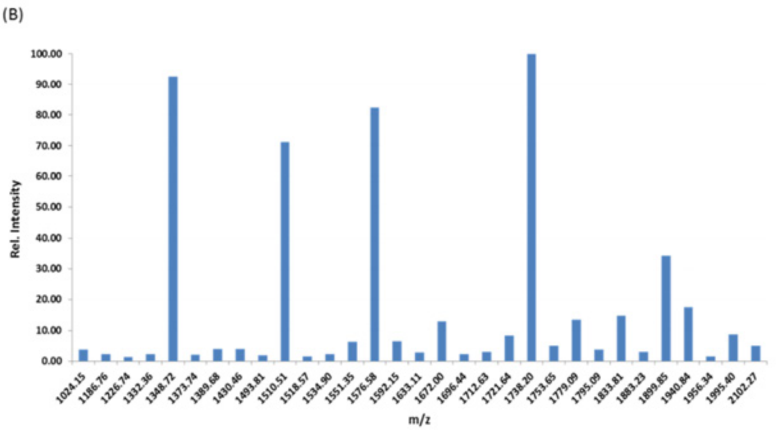
Girard's reagent T derivatization and ionic liquid matrices for improved sensitive MALDI MS analysis of N-glycans

Le Thi Hoa 오동인[1] 강철훈[*] 김태우[*]

경희대학교 동서의학대학원 [1]경희대학교 의예과

Glycans are attached in glycoprotein and play important roles in biology, those are crucial for the development, growth, functioning, or survival of the organism. For enhanced mass spectrometry detection, N-glycans are often derivatized with some hydrazine reagents to form hydrazone products, which showed the usefulness for mass spectrometric analysis. Derivatization was introduced cationic site for detection of glycans by MALDI MS. In addition, ionic liquid matrices enhance homogeneous sample, thus leading to increase MALDI-MS intensity and reduced mass background. In this study, we investigated a new method to improve sensitive MALDI TOF-MS of N-glycans using ionic liquid matrices and Girard's T reagent derivatization.





일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-28**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:21, 좌장: 하지원

Study on the solvent clusters effect on Ionization efficiency of polycyclic aromatic hydrocarbons by Atmospheric pressure photoionization mass spectrometry

이슬기다운 김성환*

경북대학교 화학과

Analytical methods have been developed for the analysis of unknown compounds in accordance with the remarkable development of modern science and the specialization of analytical instruments. However, there still remain areas that cannot be clearly defined yet. Among them, there is a remaining challenge to identify and characterize the processes of ionization in mass spectrometry. One of the important process for the ionization is interaction between solvent cluster and analyte. In this study, the effect of solvent clusters exerted on the atmospheric pressure photo ionization of polycyclic aromatic hydrocarbons (PAHs) compounds were investigated. Eight molecules having similar molecular weight but different chemical structures were dissolved into various solvent compositions and ionization efficiencies were investigated. The obtained results were compared with thermodynamic parameters derived from theoretically calculated solvent clusters. Preliminary results show that methanol clusters lower sensitivity of analysis by reacting with toluene radical ions. In case of water cluster, the reactivity with toluene radical ions was lower and hence does not affect the ionization efficiency.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-29**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:24, 좌장: 하지원

Characterization of granule in egg yolk using asymmetrical flow field-flow fractionation (AsFlFFF) coupled with multiple detectors

한수정 최재영 Lars nilsson[1] 이승호[*]

한남대학교 화학과 [1]Department of Food Technology, Engineering and Nutrition, Lund University, Sweden

Egg yolk is used in various foods such as mayonnaise, salad dressing, baking, and custard cream. Egg yolk contains soluble proteins that are called ‘plasma’ and insoluble proteins that are called ‘granule’. The plasma of egg yolk is mainly composed of low-density lipoprotein (LDL) and livetin, while the granule is mainly composed of high-density lipoprotein (HDL), phosvitin and LDLg. LDL carries cholesterol from the liver to the tissue and cell, promoting the deposition of fat in the vessel. On the other hands, HDL (‘good cholesterol’) transports cholesterol out of tissues, promoting removal of excess cholesterol in the vessel. Granule is a complex mixture of HDL, phosvitin and LDLg. They are linked through the so-called ‘phosphocalcic bridge’, and are poorly soluble in water at neutral pH. Granules are dissociated at acidic or basic pH or at high ionic strengths. Thus, in food, granules have various degrees of dissociation and conformation depending conditions such as pH or the ionic strength. In this study, we studied on how the degree of dissociation or the conformation of granules change in mayonnaise using asymmetrical flow field-flow fractionation (AF4) coupled with multi-angle light scattering (MALS). The dissociated granule components were analyzed using sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE).

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-30**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:27, 좌장: 하지원

Stable isotopic reconstructions of diets in Joseon Dynasty using human remains from archaeological site

강소영

국립문화재연구소 보존과학연구실

This study reports on human dietary reconstruction of Joseon Dynasty using stable isotope analysis. The stable carbon and nitrogen isotope values were measured of bone collagen extracted from 25 human bones from archaeological site in Myeongam-ri, Asan. Average values of δ^{13}C and δ^{15}N are –19.7±0.5‰ and 9.6±1.1‰ (*n*=23), respectively. The isotopic data indicates that Myeongam-ri individuals consumed C_3 plants mainly and assumed of dietary resourced from a terrestrial animal protein. Previous isotopic studies in Joseon period suggested that dietary composition of Joseon population was not influenced by region and burial type, but elevated δ^{15}N values in Mid-to-late Joseon era are attributed to consumption of resources from terrestrial animals. Also comparison of the isotopic results of male and female from double burials showed sex-dependent dietary patterns among individuals living in the same circumstances. These isotopic evidences have significance compared with dietary patterns of the Joseon population by various socio-economic factors and reconstruction of palaeodietary in Joseon Dynasty.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-31**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 하지원

Determination of ceramides in human skins using UPLC/Q-TOF MS and /ultra-high resolution MS

박세민 서지영[1] 김영환*

한국기초과학지원연구원 생의학오믹스연구팀 [1]충남대학교 분석과학기술대학원

Ceramides (CERs) are mostly distributed in stratum corneum (SC) of skin epidermis layer and protect from noxious external environmental such as various allergen, pathogen and water evaporation. CERs are mainly composed of total 16 subclasses (Cer [NdS, NS, NP, NH], Cer [AdS, AS, AP, AH], Cer [EOdS, EOS, EOP, EOH], Cer [OdS, OS, OP, OH]) according to variable structure and chain length of fatty acid chain, sphingosine chain and polar head group. Above all, the SC of skin almost consists of N-type and A-type CERs. The analyses of CERs species have mainly used to normal-phase (NP) LC-APCI-MS with TLC method and reversed-phase (RP) LC/Q-TOF MS. To compare change of CERs species level between health skin and atopic dermatitis skin, we performed profiling and quantification of CERs in tape-stripped SC by RP-UPLC/Q-TOF MS, 15T FT-ICR MS and orbitrap MS. The use of XBridge BEH C18 Shield column (RP column), aminopropyl (NH_2) SPE cartridge and 7.5 mM ammonium acetate increased separation efficiency and ionization efficiency of CERs species. The acquired data was analyzed by principal component analysis (PCA) and orthogonal partial least square discrimination analysis (OPLS-DA) to investigate major alteration of CERs class by atopic dermatitis.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL2.O-32**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:33, 좌장: 하지원

Molecular characterization and comparison of Asphaltenes by APPI FT-ICR and Pyrolysis-GC/HRTOF MS

진장미 김성환[1] 김영환*

한국기초과학지원연구원 생의학오믹스연구팀 [1]경북대학교 화학과

Asphaltenes are complex mixtures with polar and nonpolar compounds and have high molecular weight. Especially, there are polyaromatic hydrocarbons with containing nitrogen, oxygen and sulfur in the raw carbon residue specimens. It is important to demonstrate molecular level characterization of asphaltenes because they raise problems in petroleum industry by their undesirable properties such as uncontrolled precipitation and aggregation. In this study, the molecular characterization of asphaltene has been investigated by APPI FT-ICR MS. The overall distribution of chemical classes was determined. As a result, it was observed that S_x, O_1S_1, O_1 and HC class species were abundant. Also, the double bond equivalents (DBE) versus carbon number plots were shown for detailed information. The raw carbon residue specimens were analyzed by Py-GC/HRTOF MS in order to identify their thermally decomposed constituents. Asphaltenes were thermally desorbed at 500℃ followed by another run at 800℃ without sample handling such as dissolution or filtration. The products of pyrolysis were also characterized by chemical class distribution and DBE versus carbon number plots for main class species.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-33**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:36, 좌장: 하지원

Lipid mass fingerprinting of microorganisms by matrix-assisted laser desorption/ionization mass spectrometry

방글 김정아 김영환*

한국기초과학지원연구원 생의학오믹스연구팀

The rapid identification of bacteria is of increasing interest in food, biosafety, and clinical study. Due to rapid progress in the development of mass spectrometry devices and microorganism identification database during the last few years, bacteria identification by using mass spectrometry has become a very powerful and usable tool. We report a technique for rapid lipid profiling of bacteria by MALDI-TOF mass spectrometry. MALDI-TOF MS was applied to the rapid and direct detection of intact phospholipids from whole bacteria cells. The sample preparation procedure involved both depositing bacterial colonies directly onto the MALDI plate and using developed micro fluidic system. The phosphatidylethanolamines (PE) and phosphatidylglycerols (PG) in lipid mixture extracted from bacteria are observed in the MALDI-TOF mass spectra. The MALDI-TOF mass spectrum of each bacterial extract shows a distinguishing profile. In addition, the distinct discrimination of some species of gram negative bacteria was achieved by using principal components analysis (PCA) conducted on the relative peak intensities of phospholipids observed from the MALDI spectra. The experimental results demonstrate that the current technique is able of conducting rapid lipid analysis and has the potential for rapid clinical detection.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-34**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:39, 좌장: 하지원

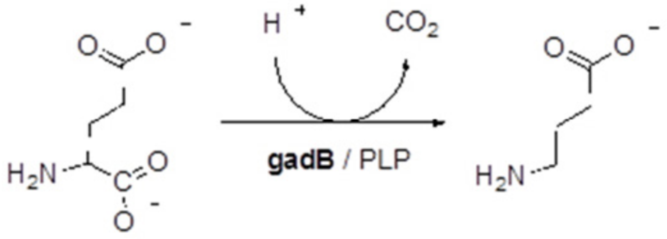
Study on oligomerization of glutamate decarboxylase (GAD) from *Lactobacillus brevis* (*L. brevis*) using asymmetrical flow field-flow fractionation with coupled multi-angle light scattering (AF4-MALS) and related techniques

<u>최재영</u> Javier Linares-Pastén[1] Lars Nilsson[2,*] 이승호[*]

한남대학교 화학과 [1]Biotechnology, Department of Chemistry, Lund University [2]Department of Food Technology, Engineering and Nutrition, Lund University

Glutamate decarboxylase (GAD) catalyzes the decarboxylation of glutamic acid giving-aminobutyric acid (GABA) (figure 1). GAD uses pyridoxal phosphate (PLP) as co-factor and H^+ as co-substrate. This enzyme is broadly present in the living organisms, from bacteria to human. GABA is one of the main neurotransmission inhibitors in nervous central system. In addition, there is increasing interest of GABA because there are evidences that it can lower blood pressure in patients with mild hypertension[1] and other potential healthy beneficial effects[2], although these mechanisms are not known yet. GABA becomes an attractive potential functional ingredient for food, but the chemically synthesized GABA is not accepted for uses in food[3]. GABA was found in some fermented food, for instance Kimchi[4], and some strains of *Lactobacillus brevis* (*L. brevis*) were identified as ones of highly GABA producers[3]. In addition, *L. brevis* is recognized as putative probiotic due potential healthy effects in humans[5]. GAD from *L. brevis* and other lactic acid bacteria apparently play an important role in the low pH resistance since it uses protons in the GABA production. It was previously reported that the highest level of activity is reached when GAD is in hexameric form and lowest when is present as dimer[6,7]. Therefore, the oligomerization seems to play an important role in the GAD mechanism. In this work we have studied the effect of pH and salt concentration in the oligomerization of a recombinant GAD from *L. brevis*, using asymmetrical flow field-flow fractionation (AF4), dynamic light scattering (DLS) and molecular modeling methods.References1. Inoue, K., et al., Eur. J. Clin. Nutr., 57, 490-495 (2003)2. Li, H. and Cao, Y., Amino Acids, 39, 1107-1116 (2010)3. Wu, Q. and Shah N. P., Crit. Rev. Food Sci. Nutr., (2016)4. Cho,

Y. R., et al., J. Microbiol. Biotechnol., 17, 104-109 (2007)5. Yakabe, T., et al., Food Chem. Toxicol., 47, 2450-2453 (2009)6. Hiraga, K., et al., Biosci. Biotechnol. Biochem., 72, 1299-1306 (2008)7. Astegno, A., Et al., Biochim. Biophys. Acta, 1854, 1229-1237 (2015)



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

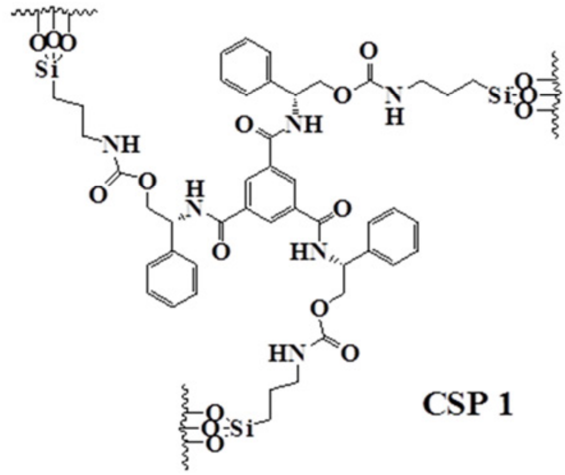
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-35**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:42, 좌장: 하지원

Synthesis and application of new (R)-phenylglycine and (S)-leucine derived C_3 symmetric HPLC chiral stationary phases

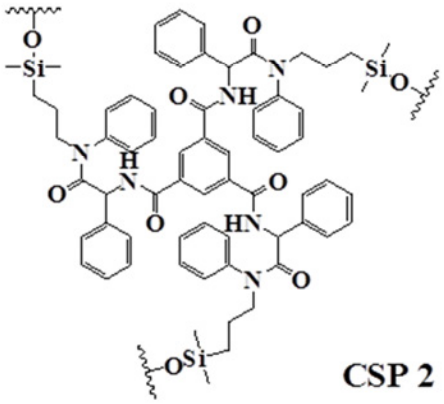
유정재 류재정[1,*]

경북대학교 화학과 [1]경북대학교 화학교육과

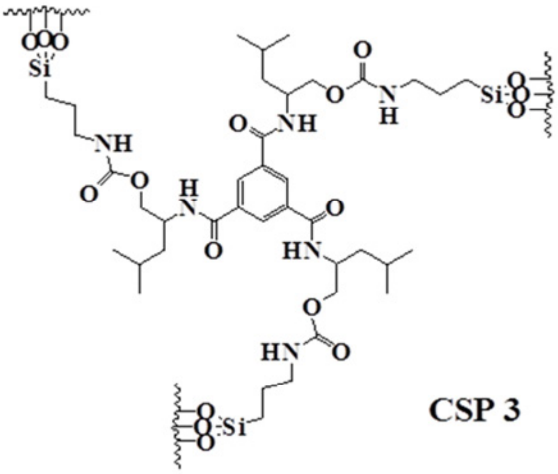
A new C_3 symmetric (R)-phenylglycinol *N*-1,3,5-benzenetricarboxylic acid derived chiral HPLC stationary phase (CSP 1) was reported recently and the CSP 1 showed good results in comparing with previously reported *N*-3,5-dintrobenzoyl(DNB) (R)-phenylglycinol derived CSP.[1] More than ten years ago, (S)-leucinol, (R)-phenylglycine and (S)-leucine derivatives were used for staring materials of 3,5-DNB based Pirkle type CSPs for chiral separation.[2,3] In this study, three C_3 symmetric CSPs(CSP 2, 3, 4) were newly prepared by the ideas and results of the three mentioned references.[1~3] The synthetic procedures and applications of the new C_3 symmetric CSPs (CSP 2 ~ CSP 4) will be shown.



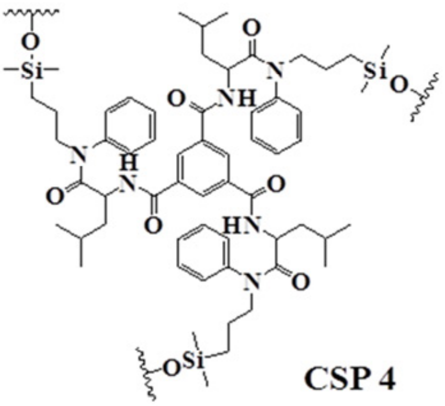
CSP 1



CSP 2



CSP 3



CSP 4

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL2.O-36**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:45, 좌장: 하지원

Development of analysis methods of Benzisothiazolinone in cosmetic products by HPLC and LC-ESI-MS/MS

하서준

식품의약품안전청 식품의약품안전평가원/화장품연구팀

Benzisothiazolinone(BIT) is known for its function as antimicrobial agent. However, BIT is currently not listed in "Inventory; Ingredients which have authorized maximum concentrations" and "AnnexV" corresponding to list of preservatives allowed in Korea and EU respectively. Therefore BIT cannot be used as a preservative in cosmetics. Besides, BIT is moderately irritating to the skin and a moderate contact sensitizer. Accordingly it is important to prevent cosmetic products containing BIT as preservative by quality control (QC) methods.In this study, we have developed well qualified analysis methods for the determination of BIT in various cosmetic matrixes. These methods have been fully validated followed by "Korean pharmaceutical method validation guideline". Quantitative method was established by HPLC and identification was set up by LC-ESI-MS/MS. The coefficients of determination() were all greater than 0.999 in the range from 0.5 to 10.0 μg/mL for HPLC and 0.02 to 5.0 μg/mL for LC-MS/MS. They showed outstanding selectivity to the cosmetic matrixes. For HPLC method, the LOD and LOQ were calculated as 0.07 and 0.21 μg/mL. In the accuracy and precision test using skin, lotion, cream and shampoo matrixes, the average recovery rate was 99.75% and the relative standard deviation (RSD) was 0.33%. On the other hand, for the LC-MS/MS method, the LOD and LOQ were 0.01 and 0.03 μg/mL, and the accuracy and precision test results were 101.50% and 3.57% respectively. We expect that the results of this study can be usefully applied in QC of cosmetic products and contributed to improve consumer safety.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.O-1**
발표분야: Oral Presentation of Young Biological Chemists
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 김석희

Discovery of Candidate Biomarkers for Type 2 Diabetes Mellitus and Vascular Stenosis and verification using selected reaction monitoring (SRM)

조경조

경희대학교 응용화학과

The major mortality of patients with type 2 diabetes mellitus (T2DM) is vascular disease like as coronary atherosclerosis. In this study, we discover and validate protein biomarker candidates for examination of vascular stenosis level using plasma samples. We consider that these biomarkers were not only cost-effective and non-invasive but also accurate sufficiently as diagnostic method of vascular stenosis. We collected the plasma samples of clinical subjects and categorize samples according to vascular stenosis level (normal, mild-to-moderate, and severe) and T2DM. Firstly, we performed identification and semi-quantification of plasma proteome using TMT-6plex reagents. We identified 1139 plasma proteins and 100 proteins were selected as differential expressed proteins (DEPs). Secondly, we performed MRM analysis without stable synthetic isotope-labeled (SI) peptides using DEPs list in small cohort (n=53). PARP4, C4A, APOC2, GC, LAMB1, CXCL7 and LBP proteins were changed significantly according to vascular stenosis level in non-T2DM subjects and IRF7, DOCK2, APOC2, HBB, LBP, CXCL7 and C4A proteins were changed significantly in T2DM subjects. Lastly, we synthesized the SI peptides according to 10 proteins and then performed MRM analysis in large cohort (n=239). On the basis of MRM results, we performed statistical analysis using t-test and ROC analysis. Interestingly, C4A, CXCL7, LBP, and GC proteins of subjects with severe stenosis significantly decreased when comparing with stenosis of normal and mild-to-moderate in non-diabetes patients group. In this result, we expect that C4A, PPBP, LBP, and GC proteins enable clinicians to diagnose the severe level of vascular stenosis in non-diabetes mellitus patients.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.O-2**
발표분야: Oral Presentation of Young Biological Chemists
발표종류: 구두발표, 발표일시: 목 09:10, 좌장: 김석희

Connecting two proteins using a fusion alpha helix and its rapid structural detection using a chemical cross linker

정우현

국방과학연구소 5본부 3부

Building a sophisticated protein nano-assembly requires a method for linking protein components in a predictable and stable structure. Most of the cross linkers available for this purpose have flexible spacers. Because of this, the linked hybrids have significant structural flexibility and the relative structure between their two components is largely unpredictable. Here we describe a method of connecting two proteins via a ‘fusion alpha helix’ formed by joining two pre-existing helices into a single extended helix. Because simple ligation of two helices does not guarantee the formation of a continuous helix, we used EY-CBS, a synthetic cross linker that has been shown to react selectively with cysteines in a-helices, to stabilize the connecting helix. After designing various fusion alpha helices, we successfully discriminate the fusion alpha helix into two groups; those which show high reactivity and those which are not. And this result of classification is well matched with the determined crystal structures – high reactivity of EY-CBS represent stable fusion alpha helix even without the cross-linking of the chemical. Our method should be applicable to detect the formation of designed alpha helix without taking full 3-dimensional structure of the target, which greatly lessen the effort for structural confirmation.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.O-3**

발표분야: Oral Presentation of Young Biological Chemists

발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 김석희

Carbohydrate Microarrays for Screening of Glycans That Stimulate the Lectin-Associated Immune Response

현지영 신인재*

연세대학교 화학과

Through binding to free glycans or glycoconjugates, animal cell surface lectins are involved in a wide range of biological processes. It has been known that most animal lectins, including selectins, siglecs (sialic acid-binding immunoglobulin-type lectins), mannose receptors, mannose-6-phosphate receptors, asialoglycoprotein receptors and C-type lectins, act as signal transducers after binding to glycans although intracellular signaling events induced by lectins depend on the nature of glycans, cell type and/or species. In particular, cell-surface lectins in the immune system bind to glycans displayed on the exterior of pathogens and this recognition event stimulates the immune response. For example, mouse SIGN-R1 (SIGN-related 1), a homolog of human DC-SIGN (dendritic cell-specific ICAM-3-grabbing nonintegrin), is highly expressed on macrophages in the splenic marginal zone and the medullar lymph nodes. This lectin binds predominantly to mannose-rich or fucosylated glycans in a Ca2+-dependent manner. Once glycans on bacterial cells or viruses interact with SIGN-R1, glycan antigens elicit SIGN-R1 mediated immune activation. As a consequence, the lectin has become fascinating markers for recognition and targeting of specific cells to regulate cellular functions and for carbohydrate-based drug discovery. To investigate glycan binding properties of cell surface lectins, we have utilized carbohydrate microarrays which allow high-throughput screening of cell-glycan interactions. Glycan microarrays used in this study were constructed by immobilizing a variety of unmodified carbohydrates onto hydrazide-coated glass slides. SIGN-R1 expressing cells pretreated with Hoechst 33342 were loaded on the glycan microarrays to evaluate the binding properties of the lectin. In addition, purified SIGN-R1 was also applied tothe microarrays for the purpose of comparison. The present study demonstrates the potential of glycan microarrays for profiling of binding specificities of cell surface lectins.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.O-4**

발표분야: Oral Presentation of Young Biological Chemists

발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 김석희

Measurement of transcriptional dynamics in living cells reveals transcription-translation coupling effects on Escherichia coli nucleoid

양소라 이남기[1,*]

POSTECH 물리학과 [1]POSTECH 시스템생명공학부/물리학

Unlike eukaryotes, transcription and translation in bacteria happen on the same space simultaneously. It has been reported that the transcription elongation rate is tightly controlled by translation rate of ribosome. However, fluorescence imaging have revealed that ribosomes are separated from the DNA and RNA polymerase (RNAP). Thus it is still unknown how the problem of spatial separation between transcription and translation is solved in living cell. Using in vivo single-molecule detection techniques, we found that the gene transcribed by RNAP is moved toward the outside of nucleoid by the translating ribosome. As a result, the transcription initiation rate is increased in living E.coli. Collectively, this cellular spatial organization by cooperation between transcription and translation play a crucial role in gene expression in E.coli.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.O-5**

발표분야: Oral Presentation of Young Biological Chemists

발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 김석희

To prevent oral bacterial adhesion on hydroxyapatite surface by coating zwitterionic MPC polymer containing calcium-binding moieties

강선아 이연*

서울대학교 화학부

The purpose of this research is to synthesize a 2-methacryloyloxyethyl phosphorylcholine (MPC)polymer which can be immobilized on the tooth surface to resist oral bacterial adhesion. To develop an MPC-based polymer with Ca2+-binding moieties, for stronger binding with hydroxyapatite (HA) of the tooth surface. For this object, a 2-methacryloyloxyethyl phosphate (MOEP) monomer was synthesized and copolymerized with MPC by free radical polymerization. The coating efficiency of the synthesized polymer, MPC-ran-MOEP with varied composition, onto a HA surface was estimated by means of contact angle measurement and XPS. The anti-biofouling property of PMP-coated HA surfaces was estimated by analyzing protein adsorption, cell adhesion, and Streptococcus mutans adhesion.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.O-6**

발표분야: Oral Presentation of Young Biological Chemists

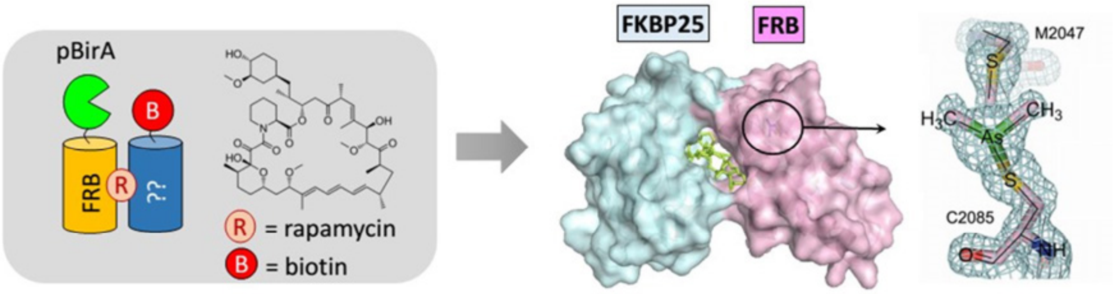
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 김석희

Proximity-Directed Labeling Reveals a New Rapamycin-Induced Heterodimer of FKBP25 and FRB in Live Cells

이송이 이현우*

UNIST 화학과

Recently, promiscuous biotin ligase (pBirA) was shown to biotin-label spatial localized proteome such as nuclear pore complex in living physiological condition. In this study, we expand to use pBirA to map spatiotemporal rapamycin-inducible interactome. Mammalian target of rapamycin (mTOR) signaling is a core pathway in cellular metabolism, and control of the mTOR pathway by rapamycin shows potential for the treatment of metabolic diseases. FKBP12 is the most well-known interacting protein to FRB domain of mTOR in presence of rapamycin. However, other rapamycin-inducible interacting protein on mTOR has not been characterized well. Thus, we tested whether FRB-pBirA could label other proteins in presence of rapamycin in living mammalian cells. After reaction, the biotinylated proteins were purified and digested, and labeled peptides were analyzed by mass spectrometry. From this analysis, surprisingly, we found FKBP25 was strongly biotinylated by FRB-pBirA in presence of rapamycin. Immunoprecipitation and immunofluorescence experiments confirmed that endogenous FKBP25 has a rapamycin-induced physical interaction with the FRB domain. Furthermore, the crystal structure of the ternary complex of FRB-rapamycin-FKBP25 was determined at 1.67-Å resolution. In this crystal structure we found that the conformational changes of FRB generate a hole where is a methionine-rich space and covalent metalloid coordination was observed at C2085 of FRB located at the bottom of the hole. Our results imply that FKBP25 might have a unique physiological role related to metallomics in mTOR signaling.From this experiment, we proposed that in vivo proteome mapping tools could be expanded to be used as an efficient method to identify drug target protein identification in living cells.


pBirA
FRB
R
??
B
R = rapamycin
B = biotin
FKBP25
FRB
M2047
S
H3C
CH3
As
S
C2085
O
NH

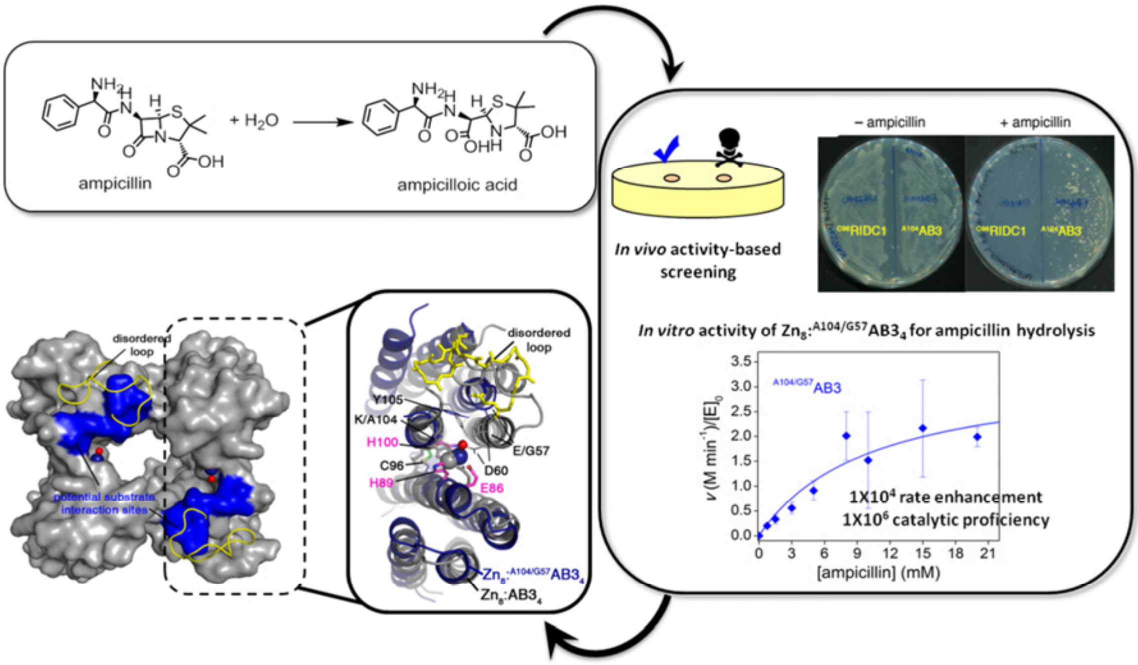
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.O-7**
발표분야: Oral Presentation of Young Biological Chemists
발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 이형호

Design of a *De Novo* Metallo-Hydrolase with *In Vivo* Activity

송윤주* **F. Akif Tezcan**[1,*]

서울대학교 화학과 *[1]Department of Chemistry and Biochemistry, University of California, San Diego*

New enzymatic activities have been primarily generated by repurposing the interiors of preexisting protein folds because designing functional, three-dimensional protein structures from first principles is a great challenge. We herein report a design of an artificial metallo-β-lactamase, constructed via the self-assembly of a structurally and functionally unrelated, monomeric redox protein, cytochrome cb_{562}, into a tetrameric assembly that possesses catalytic zinc sites in its interfaces. The designed metallo-β-lactamase ($\mathrm{Zn_8}{:}^{\mathrm{A104}}\mathrm{AB3_4}$) is functional in the *Escherichia coli* periplasm, enabling the bacteria to survive treatment with ampicillin. *In vivo* screening of ~400 mutant libraries has yielded a variant ($\mathrm{Zn_8}{:}^{\mathrm{A104/G57}}\mathrm{AB3_4}$) that displays a catalytic proficiency for ampicillin hydrolysis of 2.3 × 10^6 and features the emergence of a highly mobile loop near the active site, a key component of natural β-lactamases to enable substrate interactions. Additional mutation studies have been carried out, implying that geometric properties of the active sites might be related to the degree of protein evolution and optimization.


ampicillin
+ H2O
ampicilloic acid
− ampicillin
+ ampicillin
C96RIDC1
A104AB3
In vivo activity-based screening
In vitro activity of Zn8:A104/G57AB34 for ampicillin hydrolysis
A104/G57AB3
v (M min−1)/[E]0
[ampicillin] (mM)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
3
6
9
12
15
18
21
1X10^4 rate enhancement
1X10^6 catalytic proficiency
disordered loop
potential substrate interaction sites
Y105
K/A104
H100
C96
H89
E/G57
D60
E86
Zn8:A104/G57AB34
Zn8:AB34

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.O-8**
발표분야: Oral Presentation of Young Biological Chemists
발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 이형호

Photobleaching-free Super-resolution Fluorescence Microscopy of Living Cells

<u>심상희</u>

고려대학교 화학과

Super-resolution fluorescence microscopy opens new windows for visualizing ultrastructural dynamics in vivo. When applied to living cells, super-resolution fluorescence microscopy suffers from the limited length of time-lapse series due to high intensities of illumination and photobleaching of fluorophores. Here, I will present a new method for live-cell imaging that uses a fluorogen-binding protein, UnaG for overcoming the photobleaching limit. We found two unique photophysical properties of UnaG: (1) UnaG fluorescence is photoswitchable; (2) UnaG fluorescence can be recovered after photobleaching by replacing the damaged fluorogen with a fresh one in solution. The photoswitching property enables STORM (stochastic optical reconstruction microscopy). The ability to recover fluorescence enabled long-term STORM imaging with significant improvement in the number of independent super-resolution snapshots by 30-fold increase in STORM and 10-fold in all super-resolution methods. This method virtually eliminates the photobleaching limit due to the unlimited supply of fluorogens that can be exogenously added in solution.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.O-9**

발표분야: Oral Presentation of Young Biological Chemists

발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 이형호

Crystal structure of the multidrug transporter P-glycoprotein

진미선

GIST 생명과학부

Over-expression of the multidrug transporter P-glycoprotein is a primary mechanism for tumor cell resistance to chemotherapy. P-glycoprotein, an ATP-binding cassette (ABC) exporter, uses energy from ATP hydrolysis to translocate toxic molecules and drugs out of cells. We have determined the crystal structure of P-glycoprotein from C. elegans at 3.4 Å resolution. The protein is 46% identical to the human ortholog, and like human P-glycoprotein it confers resistance to the potent anticancer drugs paclitaxel and actinomycin D. The drug transport pathway is open to the cytoplasmic surface and also continuous with the membrane inner leaflet. Drug-binding residues identified by substrate protection are distributed over a large, mostly hydrophobic surface near the center of the membrane. Four of the twelve transmembrane segments contain perturbations of the helical secondary structure at critical junctions, possibly to mediate conformational changes associated with drug export. The interface between the transmembrane and nucleotide-binding domains, which couples ATP hydrolysis to transport, contains a ball-and-socket joint and salt bridges similar to the ABC importers. With this accurate atomic structure of P-glycoprotein, decades of functional and biochemical data can now be interpreted in molecular detail.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.O-1**

발표분야: Oral Presentations of Young Scholars in Organic Division

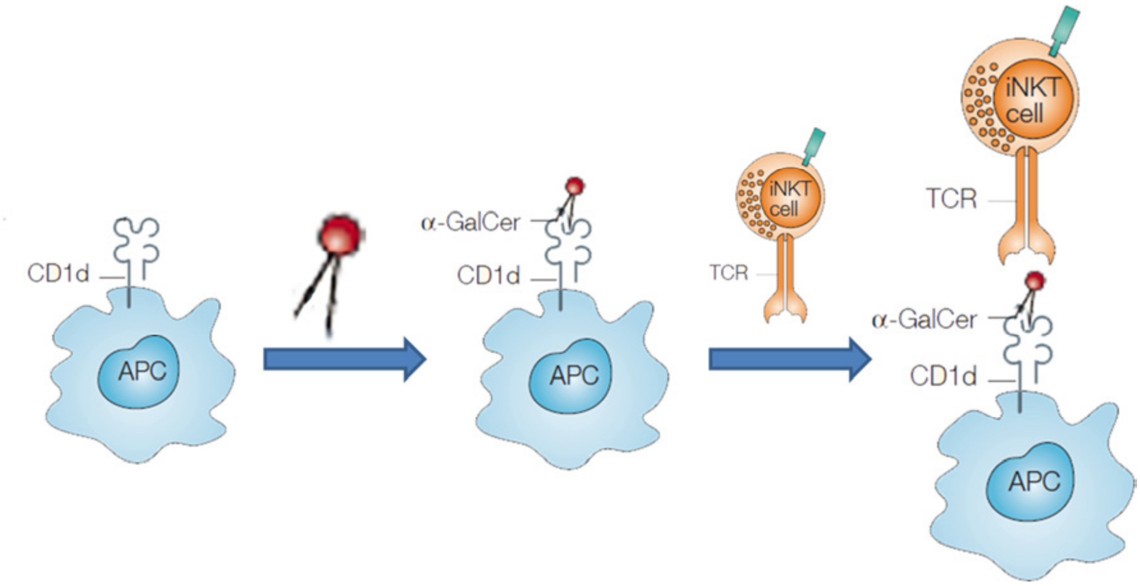
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 한순규

Development of Synthetic Pathways for α-Galactosylceramide Analogues for The Study of NKT Cell Immunity

송희범 박승범[1,*]

서울대학교 자연과학대학 화학부 [1]서울대학교 화학부

α-Galactosylceraimide (αGalCer) is a glycolipid consisting of galactose as a sugar moiety and ceramide as a lipid part linked with α-glycosidic linkage. αGalCer has received significant attention due to its immunoregularoty effect for natural killer T (NKT) cell. Once αGalCer stimulates NKT cell, NKT cell secretes various cytokines such as interferon-γ (IFN-γ), tumor necrosis factor-α, and interlukin-4 (IL-4). Recognition of αGalCer by NKT cell is mediated by antigen presenting cell (APC). First, APC binds with αGalCer through CD1d protein. Then the resulting αGalCer–CD1d binary complex is recognized by T cell receptor on the surface of NKT cell and cytokine secretion occurs. The release of cytokine by NKT cell is time dependent. For example, IL-4 is secreted maximally after 2 hour of αGalCer treatment but IFN-γ shows highest concentration around 12 hours after the treatment of αGalCer.Based on the time-dependency of cytokine secretion by NKT cell, we have focused on perturbing the binding event of αGalCer and CD1d protein in order to modulate NKT cell immune response. For the rational approach of this issue, we carefully investigated the amino acid residues in the binding pockets of CD1d protein and we found that there is an aromatic side chain-rich region in F’ pocket and cysteine-rich region in A’ pocket. Based on this structural information, we designed three different types of αGalCer analogues. First, we introduced two (hetero)aromatic rings in sphingosine backbone to induce additional non-covalent interaction with aromatic side chain residues in F’ pocket. To utilize the cysteine-rich region in A’ pocket, we introduced thiol and α-fluoroketone at the terminal position of acyl chain to make the colvant linkage with CD1d protein by reversibly and irreversibly. In addition, to identify the optimal position of newly introduced functional groups (aromatic rings, thiol and α-fluoroketone), we designed our αGalCer analogues as series having fuctional group at different position by one carbon units by one.


CD1d
APC
α-GalCer
CD1d
APC
iNKT cell
TCR
iNKT cell
TCR
α-GalCer
CD1d
APC

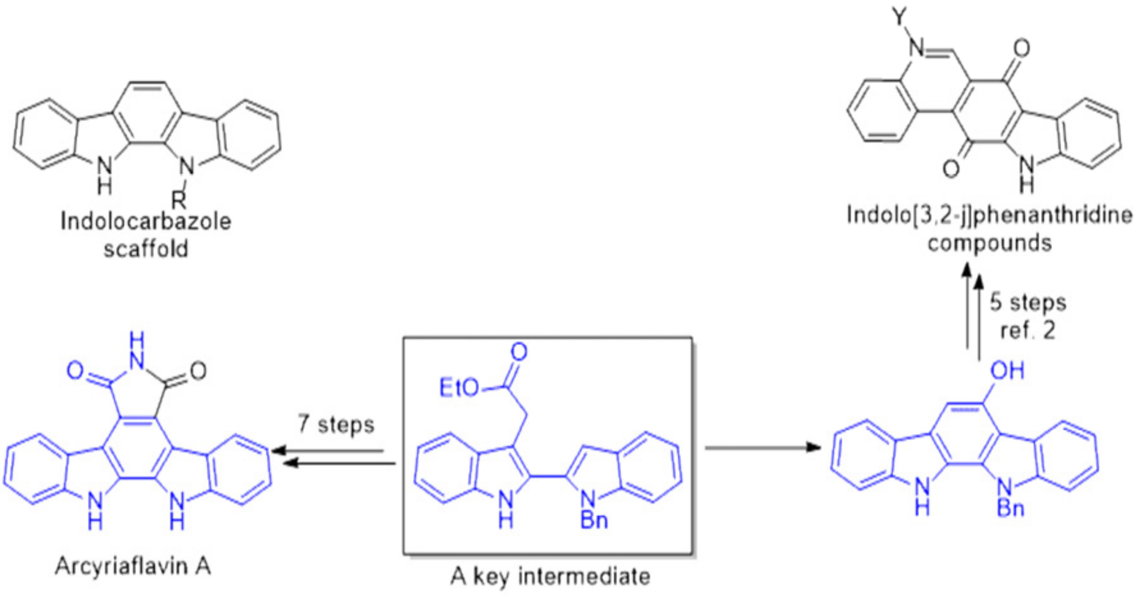
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.O-2**
발표분야: Oral Presentations of Young Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 한순규

Total Synthesis of Arcyriaflavin A and Formal Synthesis of Calothrixin B from 2,2'-Bisindole-3-Acetic Acid Derivatives via Cyanide-mediated Imino-Stetter Reaction

이성종 천철홍*

고려대학교 화학과

Since nitrogen-containing fused heteroaromatic natural products display interesting biological activities, they have drawn significant interests from the synthetic community. In addition, these natural products possess interesting and distinct structural features. For examples, arcyriaflavin A and straurosporine belong to the indolocarbazole natural products, while calothirixins A and B have indolo[3,2-j]phenanthridine skeletons. However, their previous synthetic studies have focused on developing independent synthetic routes from different starting materials, and there have been no reports on the synthesis of these natural products bearing different scaffolds from the same intermediate.Recently, we have developed an efficient protocol to access 2-arylindole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and aromatic aldehydes via cyanide-catalyzed intramolecular imino-Stetter reaction.1 Furthermore, we successfully applied this protocol to the synthesis of 2,2'-bisindole-3-acetic acid derivatives from aldimines obtained from indole-2-carboxaldehyde and (E)-2-aminocinnamaic acid derivative. Using this 2,2'-bisindole-3-acetic acid derivative as a key intermediate, we were able to finish the total synthesis of indolocarbazole natural product, arcyriaflavin A, and formal synthesis of an indolo[3,2-j]phenanthridine natural product, calothrixin B. 2 In this presentation, we will describe details in the total synthesis of arcyriaflavin A and formal synthesis of calothrixin B.References1.Lee, S. J.; Seo, H.-A.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 1566.2.McErlean, C. S. P.; Sperry, J.; Blake, A. J.; Moody, C. J. Tetrahedron 2007, 63, 10963.


Indolocarbazole scaffold
Indolo[3,2-j]phenanthridine compounds
5 steps ref. 2
7 steps
Arcyriaflavin A
A key intermediate
EtO
Bn
OH
Y
R

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.O-3**
발표분야: Oral Presentations of Young Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 한순규

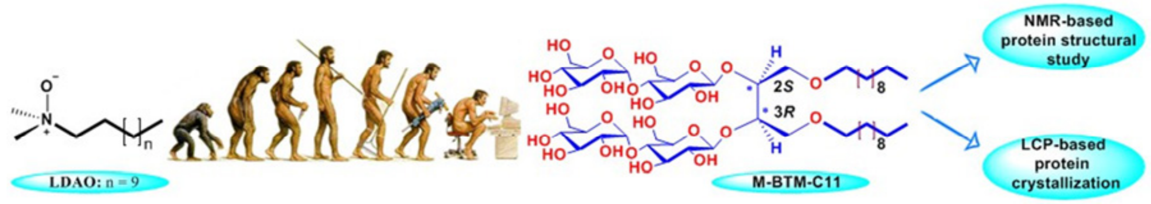
Amphiphilic Stereoisomers for Membrane Protein Study: Importance of Chirality in the Hydrophobic Backbone

DASMANABENDRA 채필석[1,*]

한양대학교 bionano engineering [1]한양대학교 생명나노공학과

Membrane proteins (MPs) are crucial cellular components, responsible for a range of key biological functions including inter- or intra-cellular material transfer and signal transduction and represent more than one-half of human drug targets. The high-resolution structures are essential to understand the underlying molecular mechanisms of these biomolecules and rational drug design efforts. Detergents are required to extract membrane proteins from the membranes and to maintain them in their native states in non-native environments. As conventional detergents have limited ability to stabilize membrane proteins, novel agents with enhanced efficacy need to be developed. Here we made efforts to develop stereoisomeric amphiphiles for membrane protein study and explore stereo-chemical outcome on stabilization of four different membrane proteins targeted here. Our collective efforts involving synthetic chemists, structural biologists and membrane protein scientists not only provide novel detergent tools useful for membrane protein study, but also include new detergent design guidelines for future development.

References:
1.M. Das, Y. Du, J. S. Mortensen, O. Ribeiro, P. Hariharan, C. J. Loland, L. Guan, B. Byrne, B. K. Kobilka, P. S. Chae, Amphiphilic Stereoisomers for Membrane Protein Study: Importance of Chirality in the Hydrophobic Region. *Chem. Sci.*, under review process.
2.M. Ehsan, Y. Du, N. J. Scull, E. Tikhonova, J. Tarrasch, J. S. Mortensen, C. J. Loland, G. Skiniotis, L. Guan, B. Byrne, B. K. Kobilka, P. S. Chae, Highly Branched Pentasaccharide-Bearing Amphiphiles for Membrane Protein Studies. *J. Am. Chem. Soc.* **2016**, *138*, 3789-3796.


LDAO: n = 9
M-BTM-C11
2S
3R
NMR-based protein structural study
LCP-based protein crystallization

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.O-4**
발표분야: Oral Presentations of Young Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 한순규

A Hollow Foldecture from the Self-Assembly of an 11-Helical Foldamer

엄재훈 공진택 권선범[1] 정록암 **Russell W. Driver**[2] 이희승[*]

KAIST 화학과 [1]Institut Européen de Chimie et Biologie, France [2]State of Hawaii Department of Health

Nature utillizes a complex ensemble of non-covalent forces to control precisely the aqueous phase self-assembly of sophisticated biological architectures. The creation of self-assembling microscale architectures that possess new and useful physical properties remains a significant challenge. Foldectures are a new class of peptidic material with unprecedented topological complexity derived from the self-assembly of foldamers. Herein we report that an 11-helical foldamer self-assembles in a controlled manner to form a series of 3D foldectures with an unusual three-fold symmetrical shapes. The foldamer packing motif was revealed by powder X-ray diffraction techniques, and provides an important link between the molecular-level symmetry and the microscale morphologies. We also demonstrated the utility of foldectures with hollow interiors as robust and well-defined supramolecular hosts for inorganic, organic, and even protein guests. We believe this work will pave the way for the design of functional foldectures with greater 3D shape diversity and for the development of biocompatible delivery vehicles and containment vessels.

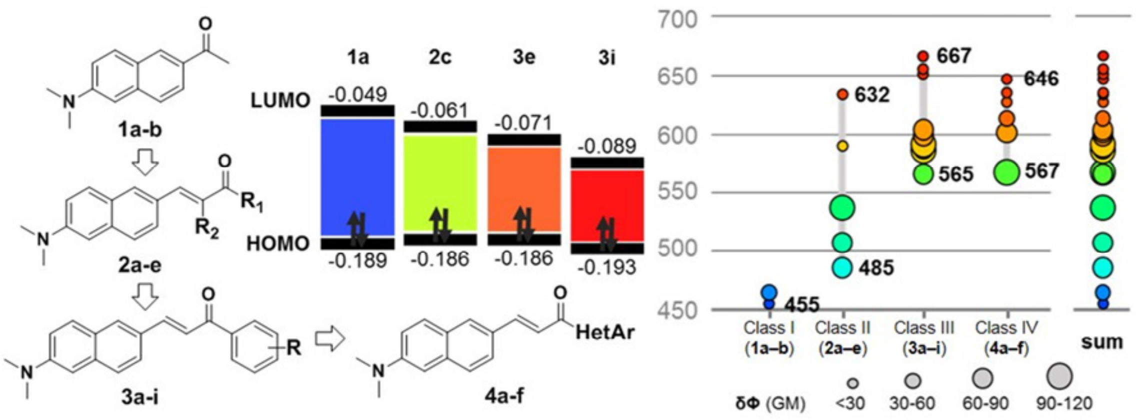
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.O-5**
발표분야: Oral Presentations of Young Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 한순규

Readily Accessible and Predictable Naphthalene-based Two-photon Fluorophore with Full Visible-color Coverage

구자영 박승범*

서울대학교 화학부

In this presentation, we reported 22 acedan-derived two-photon fluorophores with synthetic feasibility and a full coverage of visible color emission. Their emission wavelengths were well predicted by in silico analysis, which enabled us to visualize multicolor images by two-photon excitation with single wavelength, and to design a turn-on two-photon fluorescence sensor for endogenous H2O2 in Raw 264.7 macrophage and rat brain hippocampus ex vivo.



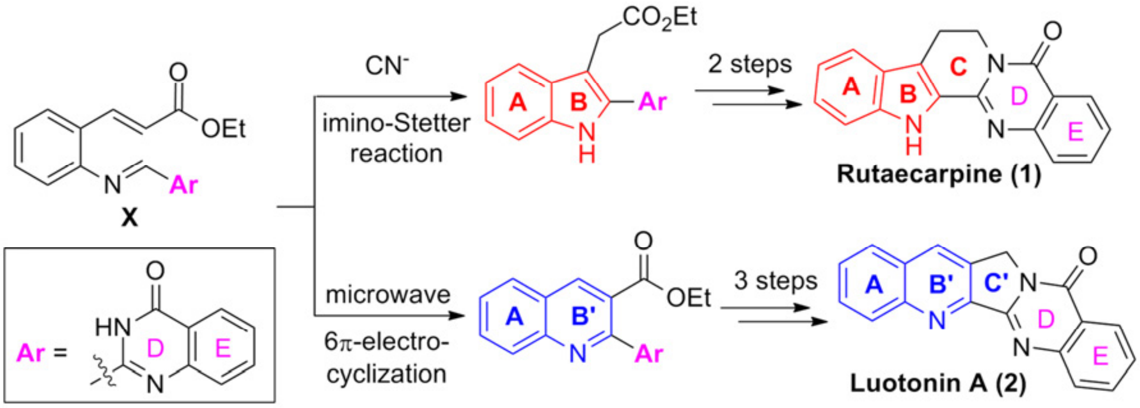
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.O-6**
발표분야: Oral Presentations of Young Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 한순규

Skeleton-Divergent Total Synthesis of Rutaecarpine and Luotonin A via the Designed Cyclization of an Aldimine

권세현 서홍안 천철홍*

고려대학교 화학과

Since quinazolinone alkaloids display interesting biological activities, a lot of efforts towards the development of new strategies for the total synthesis of quinazolinone alkaloids have been made.1 However, most of the previous approaches have focused on the synthesis of one specific target alkaloid through individual synthetic pathways, which makes them impossible to be applied to the synthesis of quinazolinone alkaloids with structural diversity. Despite structural diversities of quinazolinone alkaloids, we noticed that some of quinazolinone alkaloids have structural similarity. For instance, rutaecarpine has 5,6-membered fused rings in the B,C-rings, while luotonin A has 6,5-membered fused B',C'-ring systems, albeit both alkaloids have heterofused pentacyclic structures. Based on this structural similarity between rutaecarpine and luotonin A, we have developed the divergent synthetic pathways for both alkaloids from the same intermediate X. From the common intermediate X, 5-membered cyclization of imine in the presence of cyanide afforded the indole (B-ring) scaffold.2 Subsequent 6-membered C-ring formation led us to complete the total synthesis of rutaecarpine. On the other hand, 6-membered quinoline (B'-ring) formation via microwave-assisted thermal electrocyclization3 followed by 5-membered C'-ring formation finished the total synthesis of luotonin A. In this presentation, we describe the total synthesis of rutaecarpine and luotonin A through strategy of skeletal divergent total synthesis from a common aldimine intermediate X.4References1. (a) Lee, S. H.; Son, J.-K.; Jeong, B. S.; Jeong, T.-C.; Chang, H. W.; Lee, E.-S.; Jahng, Y. Molecules 2008, 13, 272. (b) Liang, J. L.; Cha, H. C.; Jahng, Y. Molecules 2011, 16, 4861.2. Lee, S. J.; Seo, H.-A.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 1566.3. Quinag, L. G.; Baine, N. H. J. Org. Chem. 1988, 53, 4218.4. Kwon, S. H.; Seo, H.-A.; Cheon, C.-H. Submitted.


O
OEt
N
Ar
X
Ar =
O
HN
D
E
N
CN-
imino-Stetter reaction
microwave
6π-electro-cyclization
CO2Et
A
B
Ar
N
H
2 steps
C
N
O
D
N
E
Rutaecarpine (1)
O
OEt
A
B'
N
Ar
3 steps
C'
Luotonin A (2)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.O-7**

발표분야: Oral Presentations of Young Scholars in Organic Division

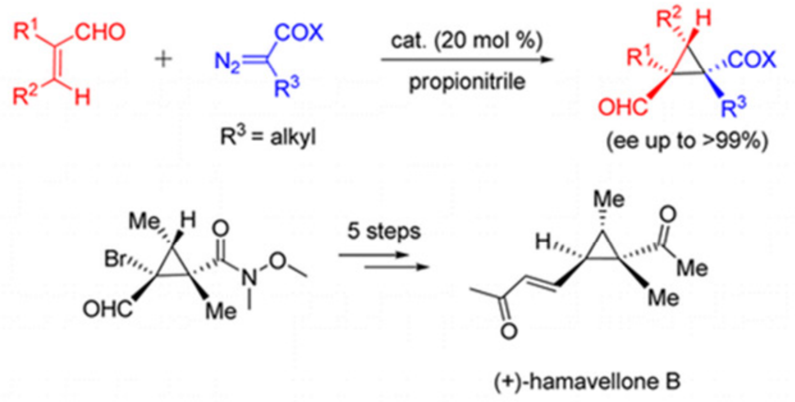
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 한순규

Enantioselective formation of small and medium size ring compounds catalyzed by chiral oxazaborolidinium ion (COBI) catalyst: Cyclopropanation and synthesis of 2,5-dihydrooxepin

심수용 류도현* 조수민

성균관대학교 화학과

Many effective cyclopropanation procedures have been described in recent years. However, the examples of asymmetric cyclopropanation of α,β-unsaturated aldehyde with diazo compounds are uncommon. In this research, we found the catalytic condition for various α-alkyl diazo compounds to provide regio- and stereoselective cyclopropanes1. The synthetic utility of this developed method was demonstrated in the first total synthesis of natural products, Hamavellone B which were isolated from soil fungus Hamigera avellanea BCC 17816. Hamavellone B was found to exhibit antimalarial activity with an IC50 of 5.2 μg/mL. Interest in the synthesis of seven-membered oxacycles has steadily increased for many years due to their occurrence in natural products, use in polymers and pharmacological applications. Because of these importance, the number of synthetic methods for the construction of seven-membered oxacycles has developed. However, there is few synthetic method of not only racemic but also chiral 2,5-dihydrooxepin. In this research, we developed enantioselective synthesis of 2,5-dihydrooxepin through retre-Claisen rearrangement of vinylcyclopropanecarboxyaldehyde.


R1
CHO
R2
H
+
N2
COX
R3
R3 = alkyl
cat. (20 mol %)
propionitrile
R2
H
R1
COX
OHC
R3
(ee up to >99%)
Me
H
Br
O
N
O
OHC
Me
5 steps
Me
H
O
Me
Me
O
(+)-hamavellone B


X
CHO
+
N2
CO2tBu
R
COBI
cat.
H
Y
X
CO2t-Bu
H
O
H
R
retro-Claisen
rearrangement
O
R
X
Y
CO2tBu

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.O-8**

발표분야: Oral Presentations of Young Scholars in Organic Division

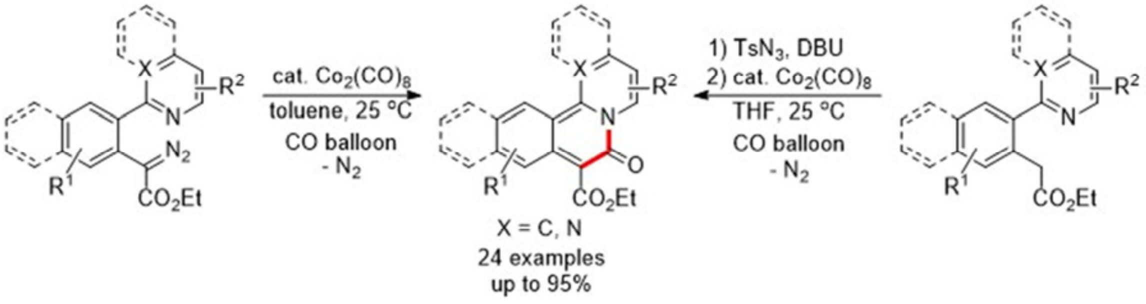
발표종류: 구두발표, 발표일시: 목 10:45, 좌장: 한순규

Co-Catalyzed Carbonylative Cyclization for the Synthesis of Pyridoisoquinolinones

백용현 이필호*

강원대학교 화학과

Dicobalt octacarbonyl-catalyzed carbonylative cyclization of pyridinyl diazoacetates is developed for the synthesis of pyridoisoquinolinones under mild conditions (room temperature) in a carbon monoxide atmosphere. Moreover, a useful synthetic method for a wide range of pyridoisoquinolinones from pyridinyl aryl acetates has been demonstrated through diazotization using TsN_3 and DBU followed by Co-catalyzed carbonylation and intramolecular cyclization of ketene with a tethering pyridinyl moiety under a carbon monoxide atmosphere in a semi-one-pot procedure. These transformations are attractive due to the use of an inexpensive and commercially available Co catalyst and an easily accessible starting material and the release of harmless N_2 under mild conditions (room temperature).This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.O-5**
발표분야: Recent Trends in Materials Chemistry
발표종류: 분과기념강연, 발표일시: 목 10:20, 좌장: 정현

Designing High-Performance, Nanostructured Carbon-Based Electrocatalysts for Renewable Energy Conversion Reactions

주상훈

UNIST 에너지화학공학부

The development of highly active and durable electrocatalysts has been of pivotal importance in renewable energy conversion and storage devices such as fuel cells and electrolyzers. Although precious group metals have been predominantly used as electrocatalysts for such devices during the last several decades, their high costs, declining activity with long-term use, and limited supplies have triggered a great deal of recent efforts toward seeking low-cost alternatives.

In this talk, I will present our recent efforts in designing nanostructured carbon-based electrocatalysts with high activity and durability for renewable energy conversion reactions, including oxygen reduction reaction, oxygen evolution reaction, and hydrogen evolution reaction. I also present our endeavor towards identifying catalytically active sites in these electrocatalysts by in situ spectroscopic and computational methods, and applying the developed electrocatalysts in system-level devices.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.O-1**
발표분야: Recent Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 신현석

Synthesis of Polybenzoquinolines as Graphene Nanoribbon Precursors

박영석* **김주환[1]** **David J. Dibble[1]** **Alon A. Gorodetsky[1,*]**

UNIST 자연과학부/화학과 [1]UC Irvine, USA

The bottom-up synthesis of graphene nanoribbons (narrow strips of sp^2 hybridized carbon) has attracted much attention in recent years, with a number of contemporary demonstrations of the preparation of all-carbon systems. However, a limited number of studies have addressed the solution-phase synthesis of heteroatom-doped graphene nanoribbons; the design and preparation of such constructs is a significant challenge. We have recently developed new synthetic methodologies for the synthesis of oligobenzoquinolines via the aza-Diels–Alder (Povarov) reaction, producing oligobenzoquinoline precursors whose length and sequence are precisely controlled. Our straightforward approach also provides access to crowded macromolecular polybenzoquinoline scaffolds, which are key intermediates for the preparation of nitrogen-doped nanoribbons. Altogether, these findings hold implications for the bottom-up synthesis of graphene nanoribbons whose edge character, terminal functionalities, doping, and length are precisely defined.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.O-2**

발표분야: Recent Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 신현석

Rational Design of Noble Metal Nanocrystals for Polymer Exchange Membrane Fuel Cell

홍종욱

울산대학교 화학

Nanocrystals (NCs) have received enormous interests in various research fields due to their distinctive electrocatalytic and catalytic activities compared to their bulk counterparts. Especially, noble metal NCs with well-defined shapes have exhibited the enhancement of electrocatalytic performances toward various electrocatalytic reactions such as methanol oxidation, ethanol oxidation, formic acid oxidation, and oxygen reduction reactions. In this regard, we have studied on synthesis of multi-metallic noble metal NCs with optimized shapes for target electrocatalytic reactions. For example, prepared octahedral Au-Pd alloy NCs showed enhanced electroactivity than the other octahedrons such as octahedral Au@Pd, Pd, and Au NCs toward formic acid oxidation. On the other hand, facet and surface area effects on electrocatalytic activities were also studied by using Au-Pd alloy NCs with high-index facets, ultrathin Pd-Pt-Ag alloy nanosheets, and Pd-Pt alloy octahedral nanocages.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.O-3**
발표분야: Recent Trends in Materials Chemistry
발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 신현석

Higher Quantum State Transitions of Colloidal Quantum Dot and Optoelectronic Applications

정광섭

고려대학교 화학과

Size-tunable bandgap, the prominent feature of the of colloidal quantum dot (CQD), has been intensively investigated for the last three decades. The size-tunable bandgap transition resulting from the quantum confinement effect that appears when the exciton is confined in the nanocrystal which is smaller than the exciton Bohr radius. To note, the quantum confinement effect is not only applied to the bandgap transition, but also to other transitions such as intraband transition occurring between the discrete electronic states in the band.

The intraband transition of CQD had been conventionally measured by using ultrafast spectroscopy due to the fast hot carrier relaxation. In this presentation, the steady-state intraband absorption and photoluminescence of mercury chalcogenides CQDs will be discussed. The air-stable steady-state intraband transition makes it possible to develop mid-infrared intraband CQD photodetector. Surprisingly, the intraband photoluminescence were observed from other II-VI system. The novel method to generalize the intraband photoluminescence of the well-known II-VI cadmium chalcogenide CQDs will be discussed as well.

1) K.S. Jeong, Z. Deng, S. Keuleyan, H. Liu, P. Guyot-Sionnest J. Phys. Chem. Lett. 2014, 5, 1139–1143.
2) Z. Deng, K.S. Jeong, P. Guyot-Sionnest ACS Nano 2014, 8, 11707-11714.
3) K.S. Jeong, P. Guyot-Sionnest ACS Nano 2016, 10, 2225-2231.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.O-4**

발표분야: Recent Trends in Materials Chemistry

발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 신현석

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

변혜령

KAIST 화학과

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

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.O-7**
발표분야: Oral Presentation in Electrochemistry
발표종류: 분과기념강연, 발표일시: 목 10:35, 좌장: 김병권

Ionics, the forgotten half-side of Electrochemistry: its role in understanding Li-ion battery electrolytes

황순욱 김동휘 이호춘*

DGIST 에너지시스템공학

Electrochemistry consists of two core fields: electrodics and ionics. Electrodics mainly deals with the charge transport at the electrified interface, while ionics concerns on the ion transport and speciation in ionic media. For the last century, the electrochemistry society has focused on electrodics with appreciable achievements, whereas ionics has seen no noticeable progress since the theory of Debye and Huckel. This indifference to ionics seems to be partly due to the misunderstanding that ionics is an old-fashioned, no-further-jobs-to-do history. Also, it may be ascribed to our relinquishment to conquer the super-complex area, obviously due to the absence of the appropriate tools and theories. However, over the past decades, we have had to confess our ignorance on the ion conduction and solution structure in the concentrated electrolytes of the energy storage/conversion devices (e.g., batteries, fuel cell, capacitors). At the same time, we have witnessed remarkable advances in the analytical instruments and computing power, which can provide us with magnificent gadgets to tackle the impregnable topic.

In this talk, as a humble first-step of the long journey toward ionics, we'll introduce some of our recent findings on the ionic conduction behaviors in the Li-ion battery electrolytes, in an association with the ion-solvent interaction as investigated using dielectric relaxation spectroscopy as well as conventional ones including Raman and pulse-field-gradient NMR.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.O-1**
발표분야: Oral Presentation in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 김병권

Non-aqueous Electrodeposition of Tantalum and Its Electrocatalytic Properties

조아라 이영미[*] 이종목[*]

이화여자대학교 화학나노과학과

Electrodeposition is one of facile methods for fabrication of electrode surface. However, electrodeposition of metal precursor in an aqueous solution is sometimes restricted by H_2O reduction. Meanwhile, nano-structured electrode often shows better electrocalalytic activity than conventional flat electrode. In this work we have carried out electrodeposition of tantalum (Ta) on carbon black loaded (Ta/CB) electrode in an acetonitrile solution. Fortunately, Ta clusters consisting of the aggregation of Ta nanoparticles (dia. ~10 nm) have been deposited on CB surfaces. Ta/CB electrode has shown a decent electrocatalytic activity for oxygen reduction in acid. In addition Ta/CB has also exhibited high sensitivity for reduction of H_2O_2 at physiological pH. To apply Ta modified electrode to biological system, Ta has been deposited on pencil lead (PL) resulting a low-cost Ta/PL electrode. Ta/PL electrode has also been used in enzymatic oxidation of monosaccharide where H_2O_2, one of the metabolic products, has been monitored in real-time.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.O-2**
발표분야: Oral Presentation in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 김병권

Interfacial Engineering in Solution-processed Inorganic-organic Hybrid Solar Cells

AMBADE SWAPNIL BALASAHEB

전북대학교 화학 공학

Organic solar cells (OSCs) are a promising photovoltaic technology due to potential for low cost fabrication based on solution-processable roll-to-roll manufacturing, their light weight, mechanical flexibility, and better efficiency in low and indirect light. One of the critical issues of OSCs has always been that of the interfaces that separates the photoactive layer and the electrodes. The electronic processes at these interfaces play a critical role in determining the efficiency for photon-to-electricity conversion. An ideal interface requires the formation of Ohmic contact with minimum resistance and high charge selectivity to prevent charge carriers from reaching the opposite electrodes. An inverted organic solar cell (iOSC) is a fascinating architecture that allows propagation of light through the thin layer of inorganic metal oxide like ZnO, which typically acts as an electron transporting layer (ETL). An ETL should necessarily posses' excellent electron transporting capabilities. In this context 1-dimensional (1D) ZnO NRs are promising candidates as they can offer ballistic transport of electrons with comparatively lesser recombinations. The synthesis of ZnO NRs mainly involves use of seeded layer to grow vertical ZnO NRs. However, the films obtained by such route are non-transparent and have poor surface coverage, especially when thinner films are required to be developed. This presentation will be focused on the use of solvothermally synthesized, low temperature processed, seedless and planar ZnO NRs as ETLs in iOSCs. The synthetic strategies along with various modification techniques like capping, doping and co-functionalization with organic small molecules, to improve the functionality of ZnO NRs for application as ETLs in iOSCs will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.O-3**
발표분야: Oral Presentation in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 김병권

Ion Conduction and Solution Structure of $LiPF_6$ and $LiBF_4$ in Propylene Carbonate Electrolytes

황순욱 김동휘 이호춘*

DGIST 에너지시스템공학

Higher ionic conductivity is indispensable property for the electrolyte to achieve higher performance of the batteries. The ionic conductivity depends not only on the ion transport property, but also on the ion association or dissociation ability of solvent in the electrolyte. However, understanding of ionics in electrolyte currently utilized for the lithium ion batteries (LIBs) is still far behind. Specifically, LiPF6 in PC solutions shows higher ionic conductivity than LiBF4 in PC solutions, while LiPF6 in PC solutions reveals higher viscosity than LiBF4 in PC solutions.Here, the ion speciation of LiPF6 and LiBF4 in PC solutions is investigated using Dielectric relaxation spectroscopy (DRS), Raman spectroscopy, and Pulsed field gradient-Nuclear Magnetic Resonance (pfg-NMR). Based on the complementary information of solution structure provided by DRS and Raman, the compositional changes of ion species are examined as a function of salt concentration. We found that LiPF6–PC solution shows higher ion dissociation than LiBF4–PC. Therefore, LiPF6-PC solution reveals higher concentration of free ion, SSIP which contribute to lithium ion transport than LiBF4–PC solution, whereas LiBF4–PC solution contains more high order salt-agglomerates which hinder the ion transport. Higher solvation number of LiPF6-PC than LiBF4–PC solution indicates that LiBF4–PC solution contains more free solvent molecules than LiPF6-PC solution and larger radius of transporting ion species in LiPF6-PC solution, leading to higher viscosity of LiPF6-PC solution than that of LiBF4–PC solution. In addition, diffusion coefficient of Li+ in LiPF6-PC is slower than that of LiBF4–PC solution because the viscosity of LiPF6-PC is higher than that of LiBF4–PC solution correlated Stokes-Einstein relation.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.O-4**
발표분야: Oral Presentation in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 김병권

Enhanced Rate Performance in Gel-Polymer Electrolyte Enabled by Reduced Li-Ion Activity

김동휘 이호춘*

DGIST 에너지시스템공학

Gel polymer electrolytes (GPEs) exhibit superior safety and dimensional stability to liquid electrolytes (LEs), which is the critical advantage in the application of Li-ion batteries (LIBs) to the large-scale applications such as electric vehicles and grid storage. The LIBs employing GPEs, however, suffer from inferior power density due to lower ionic conductivity of GPEs than LEs. In this study, it is demonstrated that the acrylate-based GPEs, prepared by in-situ thermal cross-linking polymerization, display superior rate capability to LEs. For example, LiNi1/3Mn1/3Co1/3O2/graphite cell employing the GPE exhibits 60% higher discharge capacity at 2C rate than the cell with LEs. In-depth anaylsis using three-electrode measurements, Li+ activity measurements, and Raman spectroscopy reveals that the enhanced discharge power density in GPE is due to the smaller concentration overpotential at the anode, which is ascribed to lower Li+ activity resulting from the decreased solvation number of Li+ in the GPEs.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ELEC.O-5**

발표분야: Oral Presentation in Electrochemistry

발표종류: 구두발표, 발표일시: 목 10:05, 좌장: 김병권

Silicon oxycarbide with improved electrical conductivity and lithium diffusivity for high-performance hybrid supercapacitor

HALIM MARTIN

한국과학기술연구원(KIST) 에너지융합연구단

Hybrid supercapacitors (HSCs) are recently gained a lot of attention since it takes the advantages of both high power density of supercapacitors (SCs) and high energy density of lithium-ion batteries (LIBs). HSC works by combining Faradaic reaction-based electrode from LIB and non-Faradaic reaction-based electrode from SCs. Herein, we report the investigation of silicon oxycarbide (SiOC) material in HSCs. SiOC is a ceramic material that consists of Si-O-C binding combinations such as SiO_4, SiO_3C, SiO_2C_2, $SiOC_3$, and SiC_4. High-performance SiOC was obtained by pyrolysis of phenyl-rich silicone oil. Higher pyrolysis temperature resulted in SiOC with greater electrical conductivity, which is crucial to achieving high rate capability performance. However, excessive pyrolysis temperature would result in SiOC with lower capacity. Thus, optimization is needed. Pyrolysis temperature also determines the composition of binding combinations of the SiOC. We found out that not all the binding combinations were beneficial for lithium ion storage. Among all the combinations, SiO_2C_2 is more likely to be responsible for providing lithium ion storage sites within the SiOC matrix indicated by its high capacity. Moreover, the structure of SiOC also plays an important role in providing smooth lithium ion mobilization. By employing the optimized SiOC, we successfully fabricated HSCs providing an extremely high power density of 156 kW kg^{-1} while maintaining relatively high energy density of 25 Wh kg^{-1}. In addition, the resulting HSCs demonstrated great durability demonstrated by high energy density retention of >90% even after 75,000 cycles.

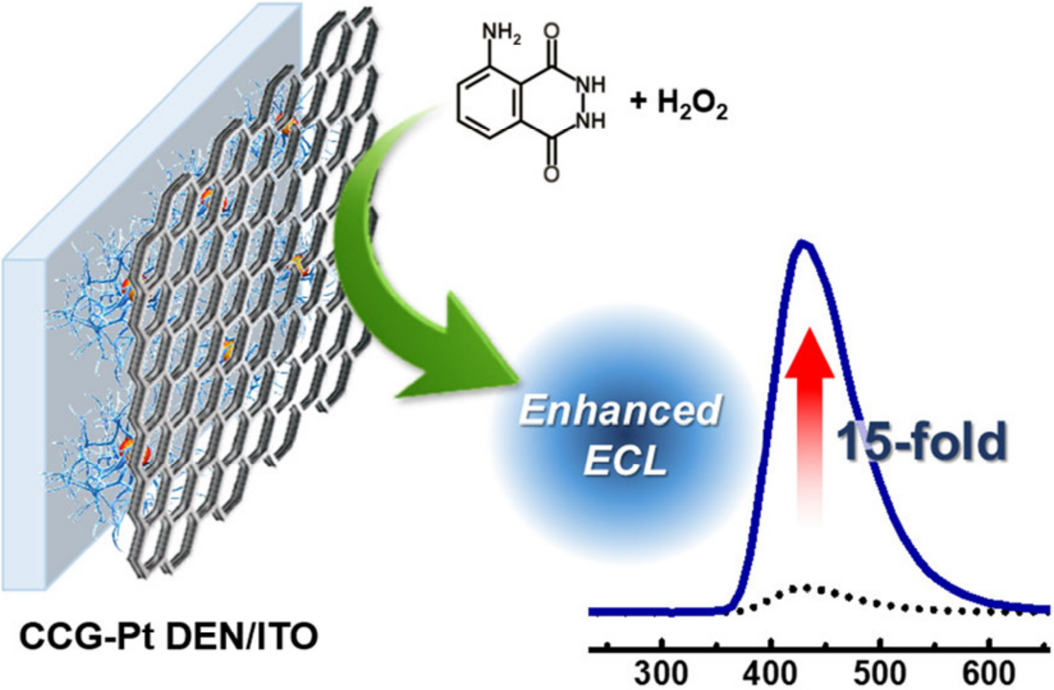
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.O-6**
발표분야: Oral Presentation in Electrochemistry
발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 김병권

Functionalization of Indium Tin Oxide Electrode with Both of Dendrimer-encapsulated Pt Nanoparticles and Chemically Converted Graphenes for Enhanced Electrochemiluminescence of Luminol/H_2O_2

조태훈 김주훈*

경희대학교 화학과

We report indium tin oxide (ITO) electrodes modified with both dendrimer-encapsulated Pt nanoparticles (Pt DENs) and chemically converted graphenes (CCGs). The modified ITOs exhibited highly enhanced electrochemiluminescence of luminol in the presence of hydrogen peroxide (H_2O_2) compared with bare ITO electrodes. We prepared Pt DENs by complexing Pt ions within dendrimers followed by chemical reduction of the complexed Pt ions. The immobilization of Pt DENs on ITO electrodes was carried out using electrooxidative grafting of the amine-terminated dendrimer-encapsulated Pt nanoparticles Pt DENs. The negatively charged GO sheets were electrostatically bound to the positively charged of amine-terminated dendrimers grafted on the ITO electrodes. The combined GO sheets were than chemically reduced to CCGs.The resulting CCG-Pt DEN/ITO electrode exhibited 15-fold enhancement of the ECL of luminol/H_2O_2 compared with bare ITO electrodes. This surface modification of ITO electrodes is of significance for the facile achievement of controllable and tunable properties of ITO electrodes for sensitive ECL-based analysis.


NH$_2$
O
NH
NH
O
+ H$_2$O$_2$
Enhanced ECL
15-fold
CCG-Pt DEN/ITO
300
400
500
600

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-1**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 김형준

Hydrogen Evolution from Multidimensional Hybrid of MoS2 and Carbon Nanotube Multilayer Thin Films

안응진 김병수[1,*]

UNIST 친환경에너지공학부 [1]UNIST 화학과

The rapid depletion of fossil fuels and growing environmental concerns have created a worldwide demand for alternative technologies of clean and renewable energies.[ref] Among many advances in the electrochemical energy conversion technology, hydrogen based fuel cell have received considerable attention as an attractive power source for next-generation energy source owing to its high energy density and environment benignity in energy generation. Molybdenum disulfide (MoS2) is a promising candidate to substitute noble metal catalysts for electrochemical hydrogen evolution from water owing to its relatively low cost, high catalytic activity and good stability.[ref] In particular, small energy variation of MoS2 in the adsorption of proton and the subsequent desorption of hydrogen during the process of HER offers a significant opportunity in developing MoS2 based electrocatalyst.However, the suspension of chemically exfoliated MoS2 sheets is often in its metastable 1T-phase, which brings the phase transition into less conducting 2H-phase or insulating oxidized MoO3 form. Thus, they often need a proper conductive support while retaining the intrinsic catalytic properties.In that regard, layer-by-layer (LbL) assembly offers a variety of opportunities for preparing multilayer thin films of desired functions with a nanometer scale control over the composition and thickness as a true nanoscale blending method.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-2**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 김형준

Beneficial Effect to Combine Metal Sulfide with Metal Oxide for Electrode Materials of Na-ion Batteries

오승미 한옥희[1,*] 황성주[*]

이화여자대학교 화학·나노과학과 [1]한국기초과학지원연구원 서울서부센터

The composite formation with metal sulfide domain makes an advantageous effect to the Na-ion electrode functionality of metal oxide. In this research, we synthesized the intimately-coupled TiO_2(B)-TiS_2 nanocomposite via the heat-treatment of TiO_2(B) under CS_2 flow. The negligible change of lattice parameters and significant enhancement of visible light absorption prove the formation of conductive metal sulfide domains. The resulting TiO_2(B)-TiS_2 nanocomposites deliver greater discharge capacities with better rate characteristics for electrochemical sodiation-desodiation process than does the pristine TiO_2(B). The role of TiS_2 domain is confirmed by ex-situ ^{23}Na magic angle spinning nuclear magnetic resonance analysis, which results clearly demonstrate that the electrode activities of the present nanocomposites rely on the capacitive storage of Na^+ ions and the TiS_2 domains in TiO_2(B)• TiS_2 nanocomposites play a role as mediators for Na^+ ions to and from TiO_2(B) domains. The present study provides clear evidence for the usefulness of in-situ composite formation between semiconducting metal oxide and metal sulfide in exploring new efficient NIB electrode materials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-3**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 김형준

Nitrogen-rich carbon nanostructure with mesoporous open channels for electrochemical energy storage applications

정형모 강정구[1,*]

KAIST KI 나노융합연구소 [1]KAIST 신소재공학과

Secondary ion batteries and various type of supercapacitors represent an important class of energy storage devices because of their high power density with a high energy density. A remarkable improvement in performance has been achieved through recent advances in the development of advanced materials. Especially, porous carbon nanostructure have their unique structural characteristics and potential applications in energy storage devices. Their novel structural properties as the electrode materials, such as abundant active sites and high ion accessibilities, are important in realizing high capacitance with robust cycle life in electrochemical energy storage applications. In this seminar, I will discuss my recent research activities on development of nitrogen-rich carbon nanostructure (NCNS) having multi-porosity for electrochemical energy storage with high performances. Through various synthetic conditions, we fabricated the unique structure, in which internal compartments enable the accommodation of numerous metal nano particles (NP) and open mesoporous channels enable fast ion insertion/desertion. Furthermore, NP embedded NCNS composite was assembled with NCNS itself into full-cell hybrid capacitor devices having an excellent rate capability and robust cycle life. We conclude that many structural advantages such as small size, porosity and ion pathway play a role as the key to success in designing the devices with high energy and high power densities.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-4**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 김형준

Nanostructured manganese oxide thin films for electrochemical supercapacitors

Bal Sydulu Singu 윤국로[1,*]

한남대학교 Chemistry [1]한남대학교 화학과

Nanostructured manganese oxide thin films were prepared by chemical bath deposition (CBD) and successive ionic layer adsorption and reaction (SILAR) methods. Nanostructured manganese oxide thin films morphology, phase of the manganese oxide and surface composition were systematically characterized by FE-SEM, TEM, XRD and XPS. The supercapacitor performance of the nanostructured manganese oxide thin film electrodes was analyzed by cyclic voltammetry (CV), galvanostatic charge-discharge (CD) and electrochemical impedance spectroscopy (EIS) method. Some of the prepared manganese oxide thin films morphology, XRD and cyclic voltammograms are shown in below Figure.

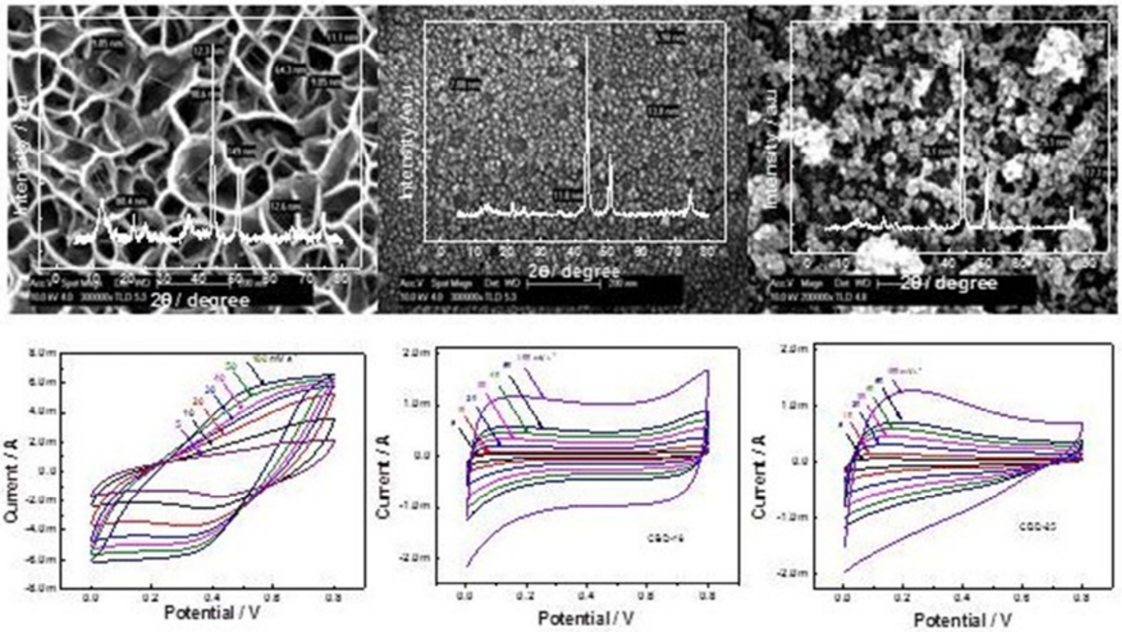


Figure 1. Morphology, XRD and Cyclic voltammograms of manganese oxide thin films prepared by chemical bath deposition.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ENVR.O-5**

발표분야: Recent Trends in Environmental and Energy Chemistry

발표종류: 구두발표, 발표일시: 목 10:10, 좌장: 정형모

Recent research trend in electrode build-up of oxidized metal composites toward achievable electrochemical conversion of carbon dioxide

이승화

GIST 지구환경공학부

Global issues of climate change and sustainable energy supplies have increased interest in the utilization of wasted carbon dioxide (CO_2) due to its carbon source for possible energy storage [1]. Among various utilization techniques, quite recently, electrochemical conversion of CO_2 into more value-added organic products by using oxidized metal electrode offers highly active, stable and selective catalytic performances [2-4]. In this presentation, previous studies and current, differing points of view on the application of oxidized metal composites to the CO_2 electroreduction are introduced. The viewpoints on the role of oxidized metal electrodes are roughly categorized into geometric or structural effects and electronic effects on the catalytic process. We hope that this introduction may inspire many research groups to become interested in the CO_2 electrochemistry, and also, lead to mutual understanding and fruitful interaction to accomplish better research prospect.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-6**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 10:25, 좌장: 정형모

A new mussel-inspired underwater adhesion mechanism and its environmental applications

김상식 황동수[1,*]

POSTECH 환경공학부 [1]POSTECH 환경대학원

It is well known that polyelectrolyte complexes and coacervates can form on mixing oppositely charged polyelectrolytes in aque- ous solutions, due to mainly electrostatic attraction between the oppositely charged polymers. Here, we report the first (to the best of our knowledge) complexation and coacervation of two posi- tively charged polyelectrolytes, which provides a new paradigm for engineering strong, self-healing interactions between polyelec- trolytes underwater and a new marine mussel-inspired underwater adhesion mechanism. Unlike the conventional complex coacervate, the like-charged coacervate is aggregated by strong short-range cation–π interactions by overcoming repulsive electrostatic interactions. The resultant phase of the like-charged coacervate comprises a thin and fragile polyelectrolyte framework and round and regular pores, implying a strong electrostatic correlation among the polyelectrolyte frameworks. The like-charged coacervate pos- sesses a very low interfacial tension, which enables this highly pos- itively charged coacervate to be applied to capture, carry, or encapsulate anionic biomolecules and particles with a broad range of applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-7**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 정형모

Enhanced Charge Reaction Kinetics of Metal-modified Hematite Photoanodes for Solar Water Splitting

전태화 최원용*

POSTECH 환경공학부

Porous hematite (alpha-Fe_2O_3) films doped with Sn(IV) and coated with an ultrathin (~2 nm thick) Nb_2O_5 passivation layer were synthesized, and the photoelectrochemical (PEC) water oxidation performance and durability of the hematite were examined in detail. As compared to hematite samples modified by either doping or passivation, dual-modified hematite exhibited a promising PEC water oxidation performance (i.e., an onset potential of ~0.7 V vs. RHE and a photocurrent density of ~2 mA cm^{-2} at 1.23 V vs. RHE in the presence of Co^{2+}) under AM 1.5 irradiation. A stable photocurrent was maintained under prolonged irradiation over 24 h, while O_2 was produced from water with a Faradaic efficiency of over 80% without showing any sign of deactivation. This performance and durability could be decoupled into separate effects of Sn doping and Nb_2O_5 layer via in-depth surface characterization and electrochemical analyses. Sn doping increased the donor density (N_d) of bare hematite by a factor of 20 and significantly improved its conductivity, leading to enhanced charge transfer efficiency. The Nb_2O_5 layer exerted an effect similar to Sn doping because of the diffusion of a fraction of Nb(V) into the hematite lattice during the annealing process at 700 ^{o}C. The primary effect of the Nb_2O_5 layer is to passivate the hematite surface and make the surface more reactive toward the oxygen evolution through water oxidation. These effects are synergistically combined in the dual-modified hematite electrode.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.O-8**
발표분야: Recent Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 10:55, 좌장: 정형모

Tantalum nitride synthesis by solution process for solar water splitting

한성규 황윤정[*]

한국과학기술연구원(KIST) 청정에너지 연구센터

광전기 화학적 촉매는 빛을 흡수하여 생성된 전하들을 활용하여 화학반응을 촉진시킴으로써 태양에너지를 화학에너지로 변환시킬 수 있다. 따라서, 태양에너지를 효율적으로 흡수하기 위한 가시광 반도체가 주로 사용되며, 물 분해 반응으로 사용되는 경우, 산환/환원 반응의 전위를 고려하여 1.8~2.0 V 의 밴드 갭이 태양광-물 분해 수소 제조 효율 10% 달성에 가장 이상적인 밴드 갭으로 제안되고 있다. 그러나 지금까지의 많은 반도체들은 합성이 용이한 금속 산화물 반도체를 활용하여 밴드 갭이 크고, 낮은 valence band 전위로 인해서 태양광-물 분해 반응에서 에너지 손실이 많음이 지적되고 있다. 질화물계열은 산화물에 비해 상대적으로 높은 valence band 를 가지고 있어 최근 각광받고 있으며, 이 중 Ta_3N_5 은 conduction band 전위가 높아 물 분해 반응에서 높은 효율을 보고 하고 있다. Ta_3N_5 는 일반적으로 Ta_2O_5 를 거쳐 합성하게 되는데, Ta 기판을 전기화학적으로 anodization 하거나 hydrothermal 반응을 통해서 Ta_2O_5 를 합성하고 있다. 하지만 이 방법은 대량생산이 어렵고, Ta 기판을 이용하기 때문에 경제적으로 좋지 못하므로 이를 대체할 용액 공정 기반 합성법을 개발하고 광전기화학적 특성을 분석하였다. 용액 공정 후, 질화과정을 거쳐 Ta_3N_5 박막이 생성됨이 SEM, XRD, XPS 등의 장비로 확인하였으며, 산소의 잔존 량에 따라 광화학적 특성이 민감하게 감소되는 것을 확인할 수 있었다. 1M KOH 용액에서 모사태양광 조건에서 최대 2mA/cm^2 (@1.6V VS. RHE)의 광전류가 얻어졌다. 합성 용액에 사용되는 Ta 전구체의 종류와 합성 조건에 따라 전하분리 효율에 크게 영향을 미쳐 광전기화학적 활성이 달라짐을, Linear sweep voltammetry (LSV), Incident photon-to-electron conversion efficiency (IPCE), Intensity modulated photocurrent spectroscopy (IMPS), Kelvin prove force microscopy (KPFM) 등의 다양한 측정방법으로 분석하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-1**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Organic photo-convertible nanoprobe hyaluronic acid-conjugated polyaniline nanocomplex for CD44-expressing cancer cells

황승연 양재문[1,*]

연세대학교 의과대학/영상의학과 [1]연세대학교 메디컬융합연구소/영상의학과

Recently, our group reported that Polyaniline (PAni) could be used to the biosensor for recognition of REDOX from cancer cells. However, PAni has a problem that is only usable in vivo environment, because PAni is difficult to give targeting capability to cancer-markers. Thus, we have designed a nanocomplex that it conjugated with hyaluronic acid (HA) as CD44-targetable biomarker, namely HA-conjugated PAni (HA-c-PAni). HA-c-PAni nanocomplexes were synthesized via the following process; reagents were dissolved in n-methyl-2-pyrrolidone, and then mixing distilled water. To confirm optical property of HA-c-PAni nanocomplexes at various pH conditions, absorbance spectra were recorded. To demonstrate physic-chemical characteristics, colloidal size using dynamic light scattering, thermal analysis using thermal gravimetric analysis, the evidence of HA-c-PAni conjugation using Fourier transform infrared spectroscopy. HA-c-PAni nanocomplexes also showed specific targeting ability for CD44-expressed cancer cells using dark field microscope. In conclusion, in this study, we synthesized HA-c-PAni nanocomplex, that exhibited a possibility of nanoprobe for biosensor, the HA-c-PAni nanocomplex can targetability and effectively detect in CD44-expressed cancer cells.Acknowledgement : This work was supported by a National Research Foundation of Korea (NRF) grant, funded by the Korean government, the Industrial Strategic Technology Development Program (10047677) funded by the Ministry of Trade, Industry and Energy (MI, Korea).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-2**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Improvement of flow-ability, chemical resistance, and weather resistance by introducing polycarbonate-polysiloxane copolymer

최진식[*] 신경무[*] 허성현[*] 정승필[*] 박정업[*] 권영도[1,*]

(주)삼양사 화학연구소 [1]삼양사 화학 연구소 기능성 소재

삼양사에서 제조되고 있는 폴리카보네이트 수지는(TRIREX) 투명성 및 기계적 물성이 우수하여 전기전자, 자동차, 광학재료분야 등에 광범위하게 사용되고 있다. 특히 TRIREX-S series 는 투명성, 저온 충격강도, 난연성 등이 우수하여 자동차 내장재 및 전기 전자 제품 하우징 재료로서 주목받고 있는 Polycarbonate-polysiloxane 공중합체이다. 최근 폴리카보네이트 소재의 용도 확대에 따라 흐름성, 내후성, 내화학성등의 고기능성이 요구됨에 따라 이와 관련하여 Polycarbonate-polysiloxane 공중합체의 흐름성, 내후성, 내화학성에 대한 개선 연구가 진행되어 왔으며 그 결과를 소개하고자 한다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-3**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Reduction Triggered Self-Cross-Linked Hyperbranched Polyglycerol Nanogel

박해리 김병수*

UNIST 화학과

Nanogels are aqueous dispersions of hydrogel particles in the nanometer range that are formed with physically or chemically crosslinked polymeric network. With their unique advantages that combine the characteristics of hydrogel and nanoparticles, nanogels are actively investigated as a promising platform for advanced biomedical applications. For this purpose, we synthesized a self-cross-linked hyperbranched polyglycerol nanogel by using thiol-disulfide exchange reaction based on a novel disulfide containing monomer. AFM, TEM, SEM, and DLS analysis successfully confirmed the tunable size and cross-linking density depending on the type of polymers (homo- or copolymer) and the amount of reducing agent, dithiothreitol (DTT). Their superior biocompatibility together with controlled release of active therapeutic agents will prospect the applicability of the nanogels in smart drug delivery systems.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-4**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Iron-Catalyzed Azidation of Polybutadiene

정해지 임영권*

국방과학연구소 4-2

Hydroxy-terminated polybutadiene (HTPB) is appropriate for prepolymer applied to binder of composite propellents due to their excellent mechanical properties, sufficient desensitization toward impact and friction, and good low-temperature elongation as well as aging characteristics. To improve the weakness of HTPB such as nonenergetic polymer, new methods for efficient and facile incorporation of energetic groups including azide, nitrite and nitramine into HTPB have attracted much attention. In this work, the research on synthesis of energetic azidated phenyl-terminated polybutadiene (AzPtPB) introduced azide groups to alkenes was described. Introduction of azide groups into PtPB was carried out by iron-catalyzed radical reaction under mild reaction conditions with low catalyst loading. Structural confirmation was conducted by FTIR, NMR and GPC analyses. Besides, thermal properties of AzPtPB were evaluated using DSC.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-5**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Novel Azo-Based Liquid Crystalline Polymers and Their Applications to Selective Alkali Metal Sensor

변인준 한양규*

한양대학교 화학과

Novel liquid crystalline polymers containing pendant azobenzene moieties with a different length of ethyleneoxy spacers were synthesized as a selective detector for alkali metal cations. Smectic structures of the azopolymers were observed by polarized optical microscope within the range of liquid crystalline phase transition temperatures. UV-Vis and 1H NMR studies confirm that the azopolymers selectively bind to Li+ and Na+, but do not complex with K+, Ba2+, Mg2+, or Ca2+. Both the ethyleneoxy spacer and azobenzene units participate in binding to Li+ and Na+ cations in solution. Interestingly, after formation of the complexed structure, the ratio of cis to trans conformer is considerably increased suggesting stronger interactions of the cis conformer with alkali metal ions. Irradiation of the complexed structure with 365 nm UV induces conversion of the uncomplexed trans to the cis. These findings suggest a great potential of the LC azopolymers as selective sensors or separation membranes for alkali metal ions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-6**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced Stability of Gold Nanoparticles by Dendrimer Capping for Surface Enhanced Raman Scattering

김광현 장지현*

UNIST 친환경 에너지 공학부

Gold nanoparticles (Au NPs) have been widely used for surface enhanced Raman scattering (SERS) due to electromagnetic mechanism well-known as surface plasmon resonance (SPR) can create an area with a huge Raman increment, called a local 'hot spot'. In this study, poly(amido amine) dendrimer was utilized to enhance the intensity and the stability of the SERS signal by encapsulating Au NPs. Dendrimer stabilized gold nanoparticles (Au-Den) were prepared by a facile solution based method for a highly reliable and robust SERS substrate. Au-Den was selectively attached on the surface of reduced graphene oxide (rGO) which was patterned with diamond shape. Au-Den/rGO exhibits the outstandingly stable and highly magnified Raman signal with an enhancement factor (EF) of 3.9 x 10^7 that enables detection of R6G dyes with concentration as low as 10 nM, retaining 95 % of the Raman signal intensity after 1 year.

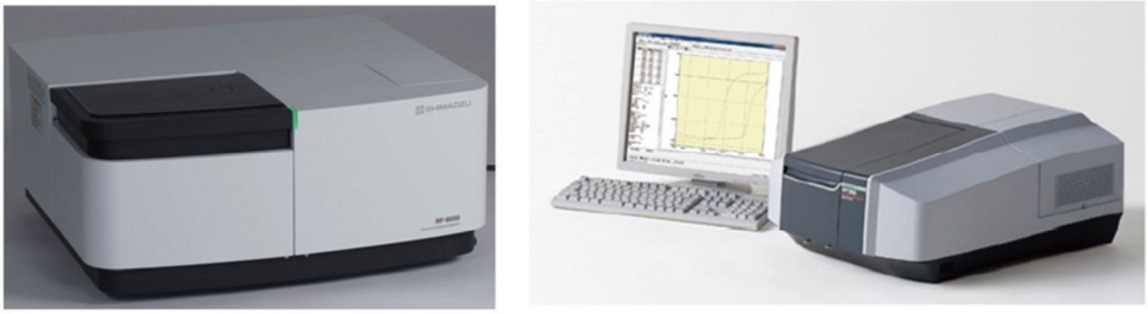
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-7**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Relative Quantum Yield Measurement of a Sample in Solution

조용주* 김관수[1,*]

동일시마즈(주) 영업지원부 [1]동일시마즈(주) 지원본부

Quantum yield can be calculated for unknown samples by a relative method that uses a fluorescent material of known quantum yield as a standard sample, or by an absolute method that uses an integrating sphere to calculate quantum yield directly(values calculated by the absolute method are called absolute quantum yield or quantum efficiency).Rhodamine B is fluorescent red pigment used to dye textiles and to color paper and other materials. A wavelength region on the excitation spectrum of uranine(sodium fluorescein) in ethanol, a substance of known quantum yield, overlaps with the excitation spectrum of rhodamine B in ethanol. Based on this, uranine in ethanol was chosen as the standard sample for calculating the quantum yield of rhodamine B. Because uranine has a peak at 498 nm(red arrow)that overlaps with the excitation spectrum of rhodamine B in ethanol, this peak wavelength was chosen as the excitation wavelength. The UV-VIS spectra of rhodamine B and uranine in ethanol are measured by using UV-2600, and Slit Width is 2 nm. Based on these spectra, at 498 rhodamine B and uranine have an absorbance of 0.0216 and 0.0243, respectively. The absorbance of both samples was ≤ 0.05, so the solutions were used without dilution to obtain emission spectra. Quantum yield program included as a standard feature of the LabSolutions RF control software for RF-6000 was used to calculate quantum yield according to formula. Required parameters for formula relating to uranine in ethanol, including quantum yield and absorbance, were entered into the formula and then the emission spectrum of uranine in ethanol was obtained. Required parameters for formula ralating to rhodamine B in ethanol were then entered into the formula and its emission spectrum was obtained. The areas of the FWHM of the peak height in each spectrum, shown in blue were calculated, and finally the quantum yield of the unknown sample rhodamine B in ethanol was calculated automatically and displayed as shown. The quantum yield program displays emission spectra with wavelength on the horizontal axis, while the FWHM area is calculated using emission spectra with values proportional to the number of photons on the vertical axis and wavenumber on the horizontal axis. Taking the quantum yield of the standard sample uranine in ethanol as 0.97, the quantum yield calculated for rhodamine B in ethanol was 0.7149, which is within the 0.69 to 0.97 range seen in literature.



RF-6000(Left), UV-2600(Right)

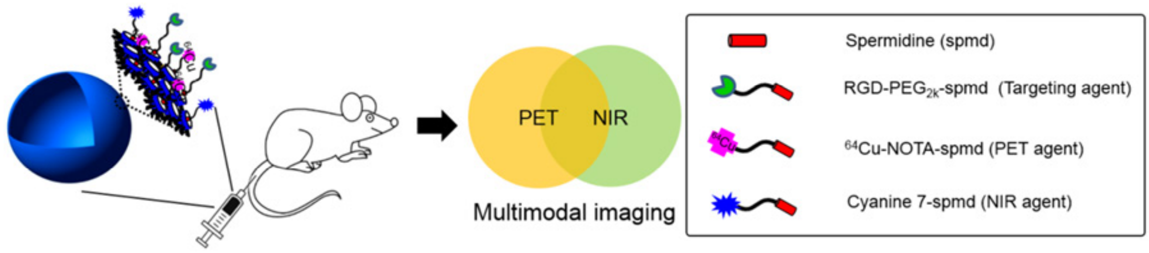
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-8**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Multimodal Imaging System Using CB[6]-based Polymer Nanocapsules as a Modular Platform

김성완 김진환[1] 김원종[1] 박경민[2] 김기문[1,*]

POSTECH 화학과 IBS [1]POSTECH 화학과 [2]기초과학연구원 복잡계자기조립연구단

Multimodal bioimaging system allows the strengths of individual imaging modalities to be combined, while complementing their limitations. This emerging imaging platform provides the potential for broad clinical imaging, for instance, early diagnosis of cancers. Nanomaterials including vesicles, micelles, nanoparticles, and nanocapsules have been utilized as promising scaffolds for multimodal imaging by modifying their surfaces with various imaging probes and targeting ligands. The modification is mostly performed by tedious, covalent approaches which often require laborious and time-consuming multistep processes. Alternatively, some noncovalent modifications using host-guest interactions of β-cyclodextrin (β-CD) to adamantane (Ad) have been reported. It, however, has an intrinsic limitation for *in vivo* applications due to the low binding affinity ($K \sim 10^4$ M^{-1}). Cucurbit[6]uril (CB[6]), a pumpkin-shaped macrocyclic host molecule, has exceptionally high binding affinity and selectivity to polyamines such as spermine and spermidine ($K > 10^{11}$ M^{-1}). Taking advantage of the unique host-guest chemistry, here we demonstrate an easily functionalizable multimodal *in vivo* imaging system using CB[6]-based polymer nanocapsule (CB[6]-PN) as a scaffold. The surface of the CB[6]-PN was successfully modified with various spermidine-conjugated functional tags in a modular manner. Utilizing ^{64}Cu-NOTA, cyanine 7, and cyclic RGDyK peptide as the functional tags for PET, NIR, and targeting, respectively, successful multimodal *in vivo* imaging of a tumor in mice suggests that the exceptional selectivity and stability of host-guest interaction of CB[6] to spermidine even under *in vivo* conditions make CB[6]PN a promising platform for multimodal imaging of cancer.


PET
NIR
Multimodal imaging
Spermidine (spmd)
RGD-PEG$_{2k}$-spmd (Targeting agent)
^{64}Cu-NOTA-spmd (PET agent)
Cyanine 7-spmd (NIR agent)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-9**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Polyimide/sepiolite hybrid films using acid activated and polydopamine-coated sepiolite

김준석 하창식[*]

부산대학교 고분자공학과

We prepared polyimide/sepiolite hybrid films. The filler loading of modified sepiolite in the polyimide matrix ranged from 2 to 8 weight percent. First, sepiolite was treated with a mixture of isopropanol/HCl solution under reflux conditions. And then the acid activated sepiolite was coated by mussel-inspired polydopamine under akaline conditions. The coated polydopamine enhanced dispersibility of sepiolite in the polyimide matrix, improving thermal and mechanical properties of polyimide composites. The modification of the sepiolite was confirmed by Fourier transform infrared spectroscopy(FT-IR), wide-angle X-ray diffraction (WAXD), field-emission scanning electron microscopy (FE-SEM) and thermogravimetric analysis(TGA). Key words: Polydopamine, Polyimide, Sepiolite, Acid activation, Hybrid film, Nanocomposite.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-10**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study of carbon black dispersion in Polyimide (PI) utilizing the multi-functional vinyl ether cross-linkers based on triphenylene core

서영범 도선정 원종찬[1] 김진수[1,*]

한국화학연구원 고기능고분자연구센터 [1]한국화학연구원 화학소재연구단 정보전자폴리머연구센터

We designed and synthesized the two novel multi-functional vinyl ether cross-linkers based on triphenylene core. Carbon black-Polyimide (CB-PI) black matrix was formulated with new cross-linkers. Optical density was measured for the CB-PI black matrix film with UV-Visible Spectrophotometer. We have studied the correlation between the chemical structure of newly developed cross-linkers and ability of dispersion of carbon black in Polyimide (PI). Also we used bispenol A divinyl ether as a control in order to evaluate the dispersion ability of carbon black of the new cross-linkers. Surface morphologies of the black matrix composite film were observed by Field Emission-Scanning Electron Microscopy (FE-SEM), Atomic Force Microscope (AFM), and Surface Profiler (α-step).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-11**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Plastic Photodetectors Based on All-Polymer Phototransistors with p-Type and n-Type Conjugated Polymers

한혜미 서주역 정재훈 김화정 김영규*

경북대학교 화학공학과

Optical sensors (photodetectors), which convert incoming radiations (from UV to IR regimes) to electric signals (current or voltage), have played a vital role in a variety of industrial and consumer applications such as healthcare systems, optical communications, security systems, personal devices, etc. Recently, photodetectors based on organic materials (small molecules or polymers) are being spotlighted as a superior alternative to rigid inorganic devices when it comes to low-cost fabrication using flexible substrates at low temperatures for wearable image sensor systems in growing flexible electronics. Of various types of organic photodetectors, organic phototransistors have attracted keen attention because they have advantages in terms of signal amplification and relatively simple/inexpensive device structures due to a triode-type configuration. In general, conventional organic phototransistors are fabricated with only single type of sensing (channel) layers, as usual for typical organic transistors, which may limit full exploitation of the benefits of organic semiconductors. In 2011, for the first time, our group has introduced “all-polymer phototransistors” with the bulk heterojunction type of channel sensing layers that consist of p-type and n-type conjugated polymers. In this presentation, we will discuss our recent advances in all-polymer phototransistors with a modified n-type conjugated polymers and briefly suggest their applications for plastic photodetectors.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-12**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Determination of the degree of cure in epoxy resins using Fourier Transform Infrared (FTIR) Spectroscopy

최미경

LG전자 소재기술원 물성분석팀

Epoxy resins have a wide range of applications such as coatings, high tension electrical insulators and adhesives. The properties of the epoxy resin mainly depend on the thermal curing process(time, temperature), and therefore monitoring the curing process has become more important than ever before. So, we focused on the determination of the degree of cure in the epoxy resins and the optimization of analysis method using Fourier Transform Infrared(FTIR) Spectroscopy. The cure reaction involves a simple addition mechanism between the epoxy ring and the amine hydrogen funtional group. The degree of cure was calculated from IR peak at 910cm-1 which depends on the epoxy rings concentrations. The epoxy resin in insulation paste was nearly fully cured about 96% when annealed at 165°C in 30min twice. Therefore, it implies that this method is quite suitable to apply on monitoring the curing process.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-13**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, characterization and properties of new conjugated conductive copolymer containing heteroatom in the main chain

조태종 김인태*

광운대학교 화학과

A new conjugated copolymer containing heteroatom in the main chain has been synthesized by stille's reaction and has good solubility in organic solvent. The copolymer was characterized by ^{1}H NMR, IR spectroscopy and UV-vis spectroscopy. The properties of the copolymer were measured by Gel permeation chromatography, UV-spectrometer, conductivity and thermogravimetric analysis. The UV-visible absorbance of the copolymer in chloroform solution shows λmax = 780 nm, hence this copolymer can be used further for solar cell devices.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-14**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on characterization and properties of the homopolymer and the copolymer containing heterocyclic compound in the main chain

김준헌 김인태*

광운대학교 화학과

New homopolymer and copolymer which have conjugated conductive properties have been successfully synthesized by direct arylation polymerization (DArP) and stille cross-coupling reaction. These polymers been characterized by ^{1}H-NMR, ^{13}C-NMR, FT-IR spectrometers. Also, the properties of the polymers have been measured by gel permeation chromatography (GPC), UV-vis spectrometer and thermogravimetric analysis (TGA). These polymers have good solubility in organic solvents such as tetrahydrofuran (THF), chloroform and chlorobenzene. These polymers also have very low bandgap. Thus, these polymers are expected to be applied to the active layer of the polymer solar cells.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-15**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Interfacial generation of iron oxide nano-flakes assembled in 2-dimensional plates for electrochemical capacitors

김아란 이선영[1] 정현민[1,*]

금오공과대학교 응용화학 [1]금오공과대학교 응용화학과

수용액층과 유기용매층 계면에서 2 차원적 판상으로 자기 조립되는 iron oxide nano-flakes 의 형성과 전기화학 커패시터로서의 성능을 평가 하였다. Iron oxide nano-flakes 는 염기성 용액과 $Fe(CO)_5$ 의 hexane 용액의 계면에서 형성됨이 관찰되었고 이들은 계면에서 2 차원적 판상으로 자기조립되었다. 반응시간을 변화시킴으로써 nano-flakes 크기를 제어하였고, 30 - 50 nm thickness 와 200 – 800 nm edge size 범위를 가지는 nano-flakes 로 자기 조립된 plates 를 조절하여 제조할 수 있었다. 이들을 커패시터 셀의 전극으로 적용하여 평가하였으며, 171 Fg^{-1} 의 우수한 specific capacitance 값을 나타내었고 정전용량의 보존은 초기 값의 85 %를 유지함으로써 비교적 우수한 사이클 안정성을 가졌음을 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-16**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of Intercalated Halloysite Nanotubes and Their Enhanced Adsorption Capability for Dye Molecules

이건구 이형욱 노재근*

한양대학교 화학과

Halloysite nanotubes (HNTs) with multi-walled structure had the original interlayer of 10 Å. To widen the inter-layer of HNTs, which called intercalation, we immersed HNTs in the saturated solution of sodium acetate (CH3COONa) and kept stirring for 3 days, 7 days, 15 days and 30 days, respectively. This kind of intercalation process can increase the volume of inter-layer about 75%. So we consider that intercalated HNTs significantly affect adsorption of dyes or other hazard molecules. In this study, we used three dye molecules such as methyl violet, malachite green and ethylene blue to investigate adsorption activity of intercalated HNTs. The resulting materials were characterized by, X-ray diffraction (XRD). Fourier transformed infrared spectroscopy (FT-IR) measurements for intercalated HNTs showed the presence of strong C=O vibration peak at 1420 cm-1, which means that HNTs were intercalated by sodium acetates. Dye adsorption was confirmed by Ultraviolet-visible spectroscopy (UV). It was found that the absorbance of dye molecules markedly decreases in the dye solution containing intercalated HNTs as a function of intercalated time. From these results, we confirmed that the intercalated HNTs were very effective to adsorption of dye.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-17**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

친환경 난연 폴리카보네이트 제조 기술 개발 (Development of New Polycarbonate Manufacturing Process)

허성현* 최진식* 정승필* 김미란[1,*] 박정엽* 신경무* 권영도[2,*]

(주)삼양사 화학연구소 [1](주)삼양사 기능성소재PG [2]삼양사 화학 연구소 기능성 소재

폴리카보네이트 수지는 내열성, 기계적 물성(특히, 충격강도) 및 투명성이 우수하여 전기부품, 기계부품 및 산업용 수지로써 광범위하게 사용되고 있다. 특히 전기전자 분야 중에서 열이 많이 발산되는 TV 하우징, 컴퓨터 모니터 하우징 등으로 폴리카보네이트 수지를 사용하는 경우에는 내열성 및 기계적 물성뿐만 아니라 우수한 난연성이 요구된다. 통상적인 방법으로 할로겐 난연제를 사용하는 경우에는 난연의 기능은 충분히 발휘되나 환경오염 문제와 더불어 연소시 발생하는 다이옥신 때문에 사용 규제 움직임이 확대되고 있다. 또한 비할로겐 난연제나 적하방지제, 금속염계 난연제 등을 사용하는 경우 투명성이 저하되는 문제가 발생한다. 삼양사에서 개발한 친환경 난연 폴리카보네이트 제조기술은 폴리실록산-분지상 폴리카보네이트 블록 공중합체를 제조하여, 난연제를 사용하지 않고도 난연성을 충분히 발휘하며, 동시에 우수한 투명성을 만족시킨다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-18**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Hydrolytic Stability of Poly(lactic acid) (PLA) / Hydrophobized Graphene Oxide (HGO) Nanohybrids

정재훈 하창식*

부산대학교 고분자공학과

Poly(lactic acid) (PLA), a biodegradable polymer, is known to be easily hydrolized under wet conditions, which has restricted its practical application. In this work, PLA nanohybrids using modified graphene oxide (HGO) were prepared by the approach of solution mixing. The Graphene oxide prepared by Hummers method was modified by octadecylamine (ODA), and it was characterized by Fourier transform infrared (FTIR) spectra and wide-angle X-ray diffraction (WAXD) patterns. The PLA nanohybrids were studied using differential scanning calorimetry (DSC), scanning electron microscopy (SEM), universal test machine (UTM), ultraviolet-visible spectroscopy, and hydrolytic degradable analysis. Homogeneous dispersion of the HGO in PLA matrix improved the hydrolytic stability in the PLA/HGO nanohybrids.

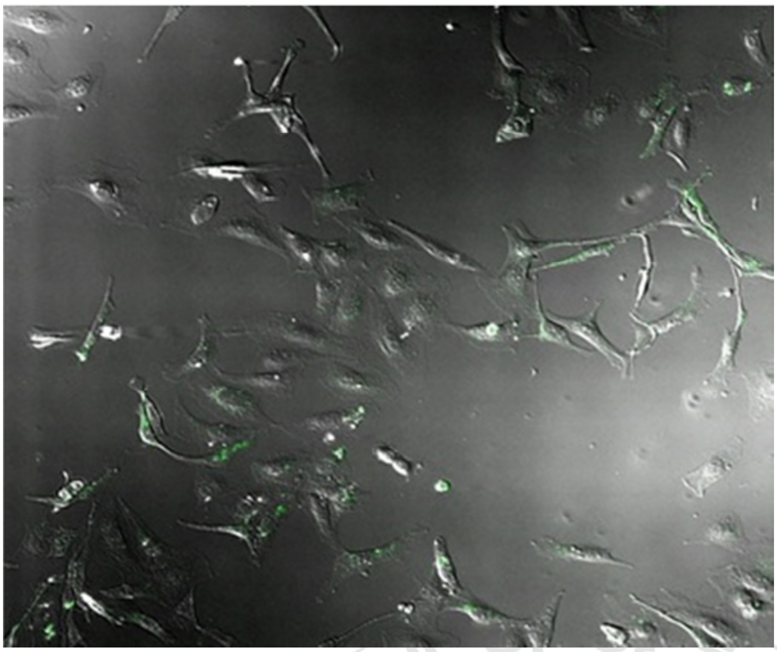
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-19**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Biodegradable L-tyrosine polyurethanes nanoparticle for gene delivery carrier

박수용 Yang H. Yun[1] 정일두[*]

부산대학교 고분자공학과 [1]Department of Biomedical Engineering, The University of Akron, USA

Polyurethane have been used as biomaterials for several decades due to their excellent physico-mechanical properties and favorable biocompatibility. A biodegradable polyurethane, which is classified as a pseudo poly(amino acid), has been developed using L-tyrosine (LTU2a). This polymer was synthesiezed using desaminotyrosyl syrosine hexyl ester, polyethylene glycol (PEG), and 1,6-diisocyanatohexane(HMDI). LTU2a is designed to degrade through hydrolysis and enzymatic mechanisms since a peptide bond since the backbone of the polymer contains a peptide bond. The successful synthesis of this polymer has been confirmed by NMR. The molecular weight and molecular distribution of nanoparticles encapsulating complexes of DNA and linear polyethylenimine(LPEI) or bovine serum albumin labeled with fluorescein have been fabricated. In addition, ther surfaces have been modified with PEG. The morphology of these nanoparticles, which was confirmed with microscopy and TEM., is spherical. The size distribution is 266 to 2500 nm. The zeta potential is -4.4 mV. The DNA release exhibited a first order kinetics. After 14 days, 15 of DNA per mg of nanoparticles have been released from the LTU2a nanoparticles. Moreover, a successful uptake of LTU2a nanoparticles by the hepatic (LX2) cells has been confirmed with confocal laser microscope, hepatic (HepG2) cells and breast (MCF7) cells has been confiremed with microscope. These characteristics are ideal for drug-devliery systems designed to transport and release drugs in the cytoplasm. Therefore, LTU2a nanoparticles could be a promising for gene-delivery applications that require sustained release of DNA for the duration of a cell's lifetime.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-20**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication and characterization of hollow PNIPAAm nanocapsules

송경주 정일두*

부산대학교 고분자공학과

In recent years, thermo-responsive polymer core-shell structures of nanometer dimensions have attracted great interest due to their potential applications. Also, polymeric hollow nanoparticles are particularly attractive functional materials due to their variety of potential applications, such as drug delivery systems, pharmaceutics, sensors, protection of biological active agents, and catalysis. In this study, thermo-responsive polymeric hollow nanoparticles were synthesized from colloidal silica (CS) and poly(ethylene glycol) methyl ether-3-(triethoxysilyl)propyl isocyanate (PEGME-IPTES) as templates for hollow and a passage connecting the inside and the outside of the hollow with N-isopropylacrylamide (NIPAAm). Silica nanoparticles were synthesized by repetition of condensation and hydrolysis of the TEOS. PEGME-IPTES was synthesized using a 3-(triethoxysilyl)propyl isocyanate (IPTES) with poly(ethylene glycol) methyl ether (PEGME) in the presence of dibutyltin dilaurate. Core-shell nanoparticles were prepared by initially coating silica with 3-methacryloxypropyltrimethoxysilane (MPS) and PEGME-IPTES, forming a shell by the polymerization of NIPAAm. Finally, thermo-responsive hollow nanoparticles were prepared by removing silica core and PEGME-IPTES by etching with hydrofluoric acid. The products were characterized by 1H-NMR, 13C-NMR, TGA, UV-vis, FT-IR spectroscopies. The particle size of products were also confirmed by using DLS, TEM.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-21**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of nanoporous hollow nanocapsules based on colloidal silica

송경주 정일두*

부산대학교 고분자공학과

Monodispersed hollow and porous polymeric nanoparticles were prepared by several step reactions. Colloidal silica core was surface-modified with 3-methacryloxypropyltrimethoxy silane (MPS) by sol-gel method, and polymerized to form crosslinked polymeric shell with styrene (St), methyl vinyl ketone (MVK) and divinylbenezene (DVB) crosslinker in dimethylformamide (DMF). Nanoporous hollow nanoparticles were prepared by photodegradation of PMVK under UV irradiation, followed by selective removal of silica core by etching with hydrofluoric acid. Hollow/porous polymeric nanoparticles were characterized by DLS, TEM, SEM image, NMR and FT-IR spectroscopies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-22**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of diol PCL-b-PLA-b-PMVK Triblock Copolymers as Biodegradable Microparticles by RAFT Polymerization

이소림 정일두*

부산대학교 고분자공학과

Biodegradable triblock copolymers based on diol polycaprolactone (PCL) were synthesized by ring opening polymerization of lactide followed by RAFT polymerization of methyl vinyl ketone(MVK). Microspheres based on triblock copolymers were prepared by emulsion-evaporation method, and then photodegraded with UV irradiation to obtain porous microparticles. In order to polymerize by RAFT method, PCL-PLA based macro-CTA (chain transfer agent) was first synthesized by reacting carboxylic acid-terminated CTA with PCL-PLA, and used to synthesize triblock copolymer with methyl vinyl ketone (MVK). The morphology of the particles before and after UV irradiation were confirmed by SEM and TEM images and the release studies of paclitaxel, anti-cancer agent for female cancers from the particles were evaluated by HPLC. PCL-PLA based biodegradable microparticles will be anticipated to enhance drug release and could find potential application for biomaterials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-23**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of Chitosan-g-poly(methyl vinyl ketone) Nanoporous Microspheres by Photodegradation for Controlled Drug Delivery System

이소림 정일두*

부산대학교 고분자공학과

Chitosan (CS) is a well-known natural polysaccharide with good biocompatibility and biodegradability. Graft copolymerization of poly (methyl vinyl ketone) [PMVK] onto chitosan was conducted by free radical method using KPS or CAN as an initiator. Nanoporous microspheres were synthesized by water-in-oil (W/O) emulsion method with glutaraldehyde (GA), Tween80®as crosslinking agent and emulsifier, followed by UV irradiation to confer nanopores by photodegradation of PMVK. Graft copolymer was characterized by FT-IR and NMR spectroscopies. SEM showed CS-g-PMVK microspheres were approximately 5 ㎛ in diameter with rough surface due to photodegradation. CS-g-PMVK could have potential applications for drug delivery system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-24**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of photocurable biodegradable surgical giude for 3D printing

신은진 정일두*

부산대학교 고분자공학과

Nowadays, photocurable resin for 3D printing is used in various field. Resins for surgical guide need strong compressive strength, wide range of workable temperature, small shrinkage and biodegradable properties. So, to get better chemical and mechanical properties, and low biodegradable property, polycaprolactone, kind of polyester, was used to synthesis of methacrylate. Polycaprolactone's characteristics give resin slow biodegradation rate and mechanical properties. Polycaprolactone trimethacrylate(PCLTMA) was analyzed with IR, GPC. To check the mechanical properties, PCLTMA is crosslinked with ultraviolet light. Camphoquinone was used for initiator and N,N'-(dimethylamino)ethyl methacrylate was used for activator. UV-cured PCLTMA's compression strength was analyzed with UTM.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-25**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Effects of Other Position of Alkyl Chain in Polymer Based on Benzodithiophene and Difluoroquinoxaline for OPVs

이원문 진영읍[1,*]

부경대학교 공업화학화 [1]부경대학교 공업화학과

PBDTT-DbiT-DFQx (in) and PBDTT-DbiT-DFQx (out) had same backbone and same alkyl side chain was introduced at other positions. The two polymers showed other optical, electrochemical, and photovoltaic properties. The result showed side chain orientation would affect to properties of the polymers. Polymers had different solubility could dissolve partially in toluene, chlorobenzene and 1,2-dichlorobenzene (o-DCB) at elevated temperature. PBDTT-DbiT-DFQx (in) indicated λmax at 538nm in CB solution and at 555 nm in thin film state, E_g^{opt} at 1.86 eV. PBDTT-DbiT-DFQx (out) showed shoulder peak in solution state and the peak intensity enhanced in film state. The shoulder peak in long wavelength happened due to the π-π* intermolecular transitions and it was caused by aggregation of the side chain. The energy level of PBDTT-DbiT-DFQx (out) lower than PBDTT-DbiT-DFQx (in). The alky sidechain ordering and hindrance were would attribute to polymer packing and altered energy levels. PBDTT-DbiT-DFQx (in) showed a highest occupied molecular orbital (HOMO) energy level of -5.21 eV, lowest unoccupied molecular orbital (LUMO) energy level of -3.35 eV, electrochemical band gap of 1.86. PBDTT-DbiT-DFQx (in) showed better V_{oc} and FF compared to PBDTT-DbiT-DFQx (out) because of good π-π stacking and effective side chain orientation. However, PBDTT-DbiT-DFQx (in) was measured poor Jsc due to the bad solubility in CB and DCB. Consequently, High 4.07% of power conversion efficiency (PCE) was achieved with PBDTT-DbiT-DFQx (in), V_{oc} of 0.67 V, J_{sc} of 9.83 mA/cm^2, FF of 0.62%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-26**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Glass-ionomer cements based using modified β-cyclodextrin

박수용 정일두*

부산대학교 고분자공학과

Glass-ionomer cements (GICs) have some advantages such as low shrinkage, low residual monomer, adhesion to the tooth directly and so on. But GICs have relatively low mechanical strength such as tensile and flexural strength. To solve the mechanical properties, resin-modified glass-ionomer cements have been developed, which provide not only the characteristics of glass-ionomer but also improved mechanical properties. Cyclodextrins(CDs) are cyclic oligosaccharides containing 6~8 glucose unit, which is can be obtained from starch by mean of enzymatic conversion. Cyclodextrins have used for food, pharmaceutical, drug delivery. Cyclodextrins have hydroxyl groups, 1 of primary hydroxyl group and 2 of secondary hydroxyl group per 1 glucose unit, which can be used chemical modification sites for varies application. In this study, β-cyclodextrin were modified by functionalities such as vinyl group and sulfonic acid or carboxylic acid. FT-IR, ^{1}H NMR, ^{13}C NMR and MALDI-TOF were used for the characterization of the modified β- cylodextrin. Glass ionomer-cements(GICs) ware prepared by photopolymerizing the modified β-cylodextrin with conventional Fuji II LC glass, compose of powder and liquid products, of various ratios. Experimental GICs were formulated by changing liquid ratio and P/L ratio to find optimal mechanical strength. Finally experimental GICs formulated by cyclodextrin derivatives with vinyl group and carboxylic acid showed highest mechanical strengths such as compressive strength(CS), diamatral tensile strength(DTS) as well as better shrinkages and viscositie.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-27**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of Modified β-Cyclodextrin with L-ascorbic acid

유은경 정일두*

부산대학교 고분자공학과

L-Ascorbic acid (AA) is one of the interesting and well known acids in nature which is used in cosmetic, pharmaceutical, and food industry due to its bioactivity and as antioxidant. But the bioavailability of AA decreases with time because it is spontaneously oxidized in the presence of oxygen. Cyclodextrin (CD) which has hydrophobic inside and hydrophilic outside, can encapsulate various organic/inorganic molecules to form inclusion complex with hydrophobic compounds. Thus they can enhance the solubility and chemical stability of such compounds in aqueous solution, and finally increase the bioavailability. This study aimed to prepare the novel skin whitening agent including CD, which has better properties in skin permeation, whitening efficiency and duration time than existing product. AA was covalently bonded to β-CD using succinic anhydride (SAH) as a linkage, and was characterized through FT-IR, NMR, DSC, TGA.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-28**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of amide-based oligomers for addtives of polyamide composites with enhanced interfacial adhesive properties

서완기 김재현 정현민*

금오공과대학교 응용화학과

폴리아마이드 강화 복합체 제조를 위한 중요 공정특성인 흐름성과 점도 특성 조절을 위해 구조가 조절된 아마이드 올리고머를 첨가제로 적용할 때 계면접착 특성이 저하됨을 방지하기 위해 본 연구에서는 아마이드 기반의 올리고머의 구조변화를 통해 컴퍼짓에서의 표면접착성 증진효과를 얻고자 하였다. 아마이드 기반의 선형 올리고머를 합성하고 이들의 말단을 조절하여 첨가제로 적용한 폴리아마이드 컴퍼짓에서의 영향을 조사하였다. 제조된 실록산 포함 말단, 카본체인의 길이가 조절된 말단 등의 아마이드 올리고머는 MALDI-TOF 및 NMR 측정을 통해 구조분석 하였고 Nylon 66 에 대해 일정한 비율로 첨가하여 컴퍼짓의 물성에 대해 상대점도, 용융점도를 확인하였으며, 아마이드 올리고머 구조가 계면 접착특성에 미치는 영향을 조사하였다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-29**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Mechanical Properties of Double Network Hydrogel

김정인

한양대학교 화학과

Double network hydrogels (DN gels) have been developed for making highly tough and elastic hydrogels. DN gels consisting of poly(N-isopropylacrylamide) (PNIPAM), poly(acrylic acid) (PAA) and inorganic clay (hectorite) were prepared by free-radical polymerization of NIPAM and AA in the presence of inorganic clay in aqueous solution. PNIPAM first network swell in the AA precursor solution and PNIPAM/PAA DN gel was synthesized by radical polymerization of PAA. The compression strength is much higher than the analogous single networks. When immersed in water, the hydrogels are opaque. The effects of the composition, such as the amounts of clay, polymer, and water content in PNIPAM/PAA DN gels on the tensile mechanical properties were investigated in detail. With increasing clay content, the modulus and the ultimate tensile strength increased, but the elongation at break decreased slightly. The tensile modulus and the strength were controlled without sacrificing extensibility by changing the clay content. By changing the polymer content, it was observed that the nature of the mechanical properties of PNIPAM/PAA DN gels changed. From the tensile and compression properties, it was concluded that a unique double network structure was retained.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-30**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Thin Film Properties of Novel Crosslinked Polyimide Gate Insulators with Ultra-Low Leakage Current Density

김의찬 안택*

경성대학교 화학과

The hydroxyl group containing polyimides (6FDA-6FHAB and DOCDA-6FHAB) were successfully synthesized with a simple one step condensation polymerization using the monomers, 5,5'-(perfluoropropane-2,2-diyl)diisobenzofuran-1,3-dione (6FDA), 5-(2,5-dioxytetrahydrofuryl)3-methly-3-cylohexene-1-2-dicarboxylic anhydride (DOCDA), and 5,5'-(perfluoro propane-2,2-diyl)bis(2-aminophenol) (6FHAB). Synthesized polyimides (6FDA-6FHAB and DOCDA-6FHAB) were further crosslinked with a poly(melamine-co-formaldehyde) as cross-linking agent. Thin film properties of novel crosslinked polyimides were systematically characterized such as chemical structures, surface roughness, surface energy, thermal stability, and capacitance, etc. Thin films of the crosslinked 6FDA-6FHAB and DOCDA-6FHAB showed good surface roughness as root mean square (rms) value as about 0.133 and 0.229 nm in AFM measurement. In addition, both crosslinked polyimide films showed extremely low leakage current densities in metal-insulator-metal (MIM) devices. The leakage current densities and breakdown voltages of crosslinked-6FDA-6FHAB and crosslinked-DOCDA-6FHAB were found to be less than 1x10-10 A/cm2 at 90 V and above 3MV/cm. Detailed synthetic routes of hydroxyl group containing polyimides and conditions of crosslinking process will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-31**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Thin Film Properties of A Thermally Curable Trifluorovinyl Containing Polyimide for Gate Insulator in Thin Film Transistor

김의찬 안택*

경성대학교 화학과

The hydroxyl group containing polyimide (6FDA-HAB) was successfully synthesized with a simple one step condensation polymerization of the monomers 5,5'-(perfluoropropane-2,2-diyl) diisobenzofuran-1,3-dione (6FDA) and 3,3’-dihydroxy-4,4’-diaminobiphenyl (HAB). And then, the hydroxyl groups of polyimide (6FDA-HAB) were further reacted with 4-(1,2,2-trifluorovinyloxy)benzoyl chloride (TFVOB) using N-methylpyrrolidone (NMP) as solvent and trimethyl amine as base. A synthesized novel polyimide (6FDA-HAB-TFVOB) was fully soluble in common organic solvents and side chains of polyimides are easily connected into the hexafluorocylobutane form by simple thermal treatment. Thin film properties of a novel crosslinked polymide (6FDA-HAB-TFVOB) were systematically investigated such as chemical structures, surface roughness, surface morphology, surface energy and capacitance, etc. The pentacene thin film transistor with crosslinked 6FDA-HAB-TFVOB as a gate insulator showed a field effect mobility as 0.25 cm2/Vs with almost no hysteresis behavior.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-32**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Study on Synthesis of Novel Conjugated Polymers by UsingFluorene and Fluorinated Quinoxaline for PSCs

이원문 진영읍[1,*]

부경대학교 공업화학화 [1]부경대학교 공업화학과

New type polymers based on fluorene and difluoro-quinoxaline were synthesized by a Stille coupling reaction and Suzuki coupling reactions, transmuting the component rate of electron-rich unit and electron-deficient unit. The polymers showed good solubility in organic solvents such as chloroform, toluene, chlorobenzene and o-dichlorobenzene (ODCB). The UV-vis absorption spectra of all polymers indicated in the range of 400 to 580 nm and maximum peak at 438 to 489 in chloroform solution and 400 to 650 nm in film. The polymers showed a highest occupied molecular orbital (HOMO) energy level in the range of -5.60 eV to -5.72 eV, and exhibit an optical bandgap of 1.98 eV to 2.16 eV. All polymers indicated good thermal stability over 400 °C. Under optimized conditions, the best efficiency among the polymers was achieved in random copolymer (ratio of 3:2) with 3.55% of maximum power conversion efficiencies, V_{oc} of 0.91 V, J_{sc} of 6.05 mA/cm_2, FF of 0.64%.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-33**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tuning the Photovoltaic Properties of Alternating Polymersby Side-Chain Engineering for OPVs

공민성 진영읍*

부경대학교 공업화학과

By altering alkyl chain length of quinoxaline unit, two donor-acceptor (D-A) type copolymers containing two parts like quinoxaline (Qx) and benzo[1,2-b;4,5-b']dithiophene (BDT) were synthesized. In order to achieve enhanced Voc , F groups with electron-withdrawing effect was introduced in the polymers . Similar UV-vis absorption in these polymers were measured in the range of 564 to 568 nm in solution and 573 to 574 nm in film state. Energy levels also displayed similar HOMO, LUMO levels and bandgap. It seems that side chain seldom influenced on optical and electrochemical properties. In photovoltaic properties, however, steric hindrance was reduced with more short side chain and it leaded to better J_{sc} of 9.66 mA/cm^2.Consequnetly, the polymer, which have a shorter side chain showed the best power conversion efficiency (PCE) of 5.11% with V_{oc} of 0.82 V, J_{sc} of 9.66 mA/cm^2, FF of 0.65%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-34**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of Fluorine Atom in New Conjugated Polymer Based on Carbazole and Quinoxaline for Polymer Solar Cells

공민성 진영읍*

부경대학교 공업화학과

A new series of solar cells (PC-DT-DFQx, PC-DT-FQx, PC-DT-Qx) were designed and synthesized. The carbazole unit was used as electron rich unit and quinoxaline unit was used as electron poor unit to make donor-acceptor type polymer solar cells. A different number of fluorine atom having electron-withdrawing effect were introduced these solar cells in order to check over the effect of fluorine atom and get more deep highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels, simultaneously. Resultingly, in electrochemical properties, these polymers showed HOMO levels of -5.44,-5.48 and -5.58 eV and the LUMO levels of -2.94, -2.97 and -3.30 eV, respectively. Among the polymers, The polymer PC-DT-DFQx displayed a highest value of 5.06% power conversion efficiency (PCE) and value of 0.85 V open-circuit voltage (V_{oc}).

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-35**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Two New D-A Type Copolymer through Di-Fluorinated Quinoxaline and Indacenodithiophene for PSCs

공민성 진영읍*

부경대학교 공업화학과

The new D-A type alternating copolymers (PIDT-DFQx, PIDT-DTDFQx) with low band gap were synthesizyed by polymerization such as a Stille coupling reaction using Pd catalyst. Indacenodithiophene (IDT) unit containing a alkyl phenyl group was used as an electron-rich unit, Whereas Di-fluorinated quinoxaline (DFQx) was used as an electron-deficient unit. In order to look into influence of thiophene bridge, either DFQx or thiophene substituted DFQx on both side was designed and synthesized. Two polymers showed strong absorption in the range of 558- 576 nm in solution state. PIDT-DTDFQx ,which have a thiophene bridge displayed broader absorption than those of none. Resultingly, these polymers displyed 0.93%, 2.87% of power conversion efficiency (PCE), respectively.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-36**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Properties of Novel Thiophene Copolymer with Fluorine Substituted Quinoxline for PSCs

정동환 진영읍*

부경대학교 공업화학과

Novel copolymer consist of difluoro-quinoxline (5,8-dibromo-2,3-didodecyl-6,7-difluoroquinoxaline) and mono fluoro-quinoxaline (5,8-dibromo-2,3-didodecyl-6-fluoroquinxaline) was synthesized by stille and Suzuki coupling reaction for use in polymer solar cells. In these polymers, quinoxaline unit was used as electron-deficient unit and thiophene unit was used as electron-rich unit. These polymers have poor solubility in common type of organic solvents such as chloroform, toluene, chlorobenzene and o-dichlorobenzene (ODCB). The thermal stabilities of polymers were investigated using thermogravimetric analysis (TGA). The decomposition temperatures (T_d) at 5% loss of these polymers was observed over 390℃ under an inert nitrogen. A highest molecular orbital (HOMO) energy level was indicated in the range of -5.28 ~ -5.47 eV. The polymers have absorption in the range of 450 ~ 700 nm.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-37**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study of reactivity of monomers with functional groups for polyphenylenesulfide copolymers

<u>김관수</u> HOTHINGUYETLINH[1] 정현민[1,*]

금오공과대학교 응용화학화 [1]금오공과대학교 응용화학과

p-디아이오벤젠 (PDIB)에 대한 황의 직접반응을 통해 설파이드 결합을 형성하여 폴리페닐렌설파이드(PPS)를 중합하는 신공정이 연구되고 있으며 이러한 중합법에서 PPS 물성 개선과 다양화를 위해 기능기를 포함하는 단량체를 도입한 공중합체 제조도 관심의 대상이 되고 있다. 방향족 아이오다이드 화합물에 대한 황의 직접 반응조건에서 기능기를 갖는 단량체의 반응성과 안정성에 대해서 디페닐디설파이드(DPDS)를 황 대신 적용하는 모델반응을 통해 공중합 조건에서의 특성을 조사하였다. 전자끄는기 및 전자주는기 등 다양한 기능기를 갖는 디아이오도 화합물의 반응 경향성을 파악하였으며, 디아이오도 화합물중 디아이오도벤조산(DIBA)과 반응한 생성물을 통해 황 라디칼 농도에 따른 카르복시 그룹의 안정성, 그리고 디아이오도페닐설폰(DIPS)의 반응성을 1H NMR 및 FT-IR 을 통해 모니터링하여 분석하였다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-38**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of Thienyl Group in Alternating Polymers Based on Benzodithiophene and Quinoxaline Unit for Photovoltaics

정동환 진영읍*

부경대학교 공업화학과

The new type conjugated polymers (BDT-T-FQx, BDT-T-DFQx, BDT-T-DTFQx, BDT-T-DTDFQx) based on thienyl substituted benzodithiophene (BDT-T) and mono- or di- fluorinated quinoxaline (Qx) derivatives were designed and synthesized. BDT-T unit was used as electron-rich unit and Qx unit was used as electron-deficient unit. One or two fluorine group was introduced in acceptor unit to achieve more low bandgap. These polymers had a good thermal stability with 5% weight loss temperature over 320℃. Maximum absorption peak was measured at 560~620 nm in solution and 570~627 nm in solid thin film in these polymers. And in solid thin film, red-shift was observed because of stronger intermolecular interaction. These polymers showed HOMO energy level -5.39, -5.45, -5.24, -5.32 eV and LUMO energy level -3.55, -3.58, -3.38, -3.43 eV, respectively. Consequently, Among these polymers BDT-T-DTFQx achieved highest PCE 5.95% with 11.76 J_{sc} value , 0.74 V_{oc} value and 0.68 FF.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-39**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tactic to Make Regioregular Conjugated Polymers Based on Mono-Fluorinated Quinoxaline Unit for Photovoltaics

정동환 진영읍*

부경대학교 공업화학과

Regiochemistry is one of the most promising tactics to improve the efficienty of PSCs. The new conjugated polymers (BDT-DTFQx (80℃), BDT-DTDFQx (50-80℃)) was synthesized by controlling temperature to make polymers regioregular. Benzodithiophene (BDT) was used as electron-rich unit and quinoxaline (Qx) was used as electron-deficient unit. These polymers had a good thermal stability with 5% weight loss temperature over 320℃. These polymers displayed maximum absorption peak at 546~567 nm in CB solution and at 576~579 nm in film state, more red-shift was observed in BDT-DTDFQx (50-80℃) because it had more regioregular orientation than BDT-DTDFQx (80℃). And these polymers showed similar HOMO energy level and LUMO energy level due to same backbone of polymers. As a result, BDT-DTDFQx(50-80℃) had more high PCE 5.73%

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-40**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of energetic polymer containing ferrocene

정지혜 임영권*

국방과학연구소 4-2

Glycidyl azide polymer(GAP) has been used for energetic binders. GAP has good properties such as low T_g, low viscosity, high density, high positive heat of formation, and good compatibility with eco-friendly oxidizers. Ferrocene derivatives have been widely used burning rate catalyst for propellants. To make energetic binder which are improved burning rate, we designed poly(glycidyl azide-co-glycidyl ferrocenyl ether)(PGAFE)s are synthesized by three step reactions. The structures of PGAFTs are confirmed IR, ^{1}H and ^{13}C NMR spectral analyses. Thermal properties of the PGAFEs are evaluated using differential scanning calorimetry (DSC).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-41**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Spiropyran 분자 센서를 통한 계면에 따른 stress 전달

김종찬

한국과학기술연구원(KIST) 다기능구조용연구센터

스파이로파이란은 기계적 활성을 갖는 메카노포의 한 종류로써, 다양한 외부 자극(힘 또는 자외선)에 의해 SP form 에서 MC form 으로 변환된다. 일반적으로, 스파이로파이란은 닫힌 고리 구조(SP form)이지만, 인장시 약한 C-O 결합이 깨지는 개환 반응을 통해 메로시아닌(merocyanine) form 으로 변한다. 또한 가시광선에 의해 가역적으로 다시 닫힌 고리 구조로 변환된다. 거시적으로 스파이로파이란은 열린 고리 구조에서 옅은 노란색으로 보이며 닫힌 고리 구조에서 짙은 보라색을 띤다. 이와 같은 광 변색현상(photochromism) 특성으로 스파이로파이란은 스트레스 탐색 분야, 고분자/복합소재 역학 분야, 센서 분야 등에 널리 연구되고 있다.본 연구에서 우리의 목표는 E-glass fiber 및 고분자 표면에 SP 분자를 도입하여 다른 종류의 계면력(van der Waals vs. covalent)을 시각적으로 비교, 분석하는 것이다. 두 종류의 SPs(di-functional and mono-functional)를 합성하였다. Di-functional SP 는 E-glass fiber 와 고분자 표면에 SP 를 공유 결합으로 연결한 모델인 반면에 mono-functional SP 의 경우 E-glass fiber 의 말단기에만 화학적 결합을 형성하여 고분자와 SP 사이에 Van der Waals 를 연구하는 모델이다. 최종적으로 기계적 활성을 갖는 SP 의 특성은 opto-mechanical system 인 계면 전단 강도 시험(interfacial shear strength test)과 형광 강도 측정을 이용하여 분석하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-42**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of electroconductive hydrogels by UV-mediated thiol-ene reaction

최은정 송창식* 송선구 김경수

성균관대학교 화학과

Thiol-ene reactions have been widely used because they have the characteristics of “click reactions”, which are fast and high-yielding without side reactions. The hydrothiolation reactions proceed either by a radical pathway or catalytic pathway. Although there are differences of reactivity and reaction mechanism, ene species (i.e. terminal alkene, norbornene) and thiol species have a wide range of substrate scope to proceed thiol-ene reaction. In this study, alkene-functionalized alginates were converted to hydrogels via UV-mediated thiol-ene reaction. For furnishing electroconductivity, the alginates were blended with conducting polymers. The synthesized hydrogels were characterized by rheology and electrochemical spectroscopy. We tested the electoconductivity of the hydrogels when divalent ions are bound to alginate, since the microstructure of the hydrogel can be changed upon binding of divalent ions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-43**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

In-situ synthesis of conjugated polymer/gold nanoparticle hybrids : solvent and molecular-weight effects

송창식* 하성균 이주경 송선구

성균관대학교 화학과

The gold nanoparticle/conjugated polymer hybrids are well known for their enhanced electrochemical, physical, optical and chemical properties than separated composites. These enhanced properties can be used in various fields as surface-enhanced Raman scattering, sensors, heterogeneous catalysis, solar cells, and memory devices. For these applications, precise control of shape and size of gold nanoparticle/conjugated polymer hybrids materials is very important. Here, we designed binaphthyl-incorporated conjugated polymer for reduction and stabilization of gold nanoparticles to form nano hybrid materials. We found that the polymers with different molecular weights and solvents have different hydrodynamic radius. The larger hydrodynamic radius of the polymers made branched bigger gold nanoparticle/conjugated polymer hybrids and smaller hydrodynamic radius made the smaller, sphere-like shape gold nanoparticle/conjugated polymer hybrids; due to the coverage of gold nanoparticles facets is different. The synthesized gold nanoparticle/conjugated polymer hybrids showed the enhanced electrochemical properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-44**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Self-assembled photo-catalytic systems using metal-terpyridine interaction

정동철 이주경 송선구 송창식*

성균관대학교 화학과

Photo-active polymers are one of the most important materials because of their potential applications in solar energy conversion and photo-catalytic system. In this study, we synthesized a polymer and a ruthenium complex, both of which are functionalized with terpyridine (tpy). The tpy ligand in the polymer and ruthenium complex can bind to metal ions (e.g., Fe^{2+}, Zn^{2+}, Co^{2+}, and Mg^{2+}). With the ruthenium complex and Mg^{2+} ion, we confirmed photocurrent generation after assembly on tpy-coated ITO substrates. When Mg^{2+} ions were removed by using tetra-n-butylammonium fluoride (TBAF), the assembled polymeric complex underwent decomposition and the photocurrent decreased. However, the photocurrent efficiency of this system can be recovered through re-assembly, and repeated several times without significant decrease of its efficiency. Additionally, the assembled polymer complexes can be used as a photocatalyst that convert benzylamine to imine by photo-oxidative coupling. The photocatalytic system produced the imine compound after assembly, but when TBAF was added for disassembly, the system showed no reaction due to the removal of the ruthenium complex. The self-assembly of photocatalytic systems will enable self-repairable photoactive materials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-45**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Self-Assembly of Thermoresponsive Microgel Particles by Metal Terpyridine Interaction

이주경 송창식* 정동철 최은정

성균관대학교 화학과

pNIPAM has temperature-responsive property that it collapses when heated above the lower critical solution temperature (LCST) in water. Due to their unique features, pNIPAM-based microgels have been suggested as promising materials in several potential applications such as drug delivery, biosensor and chemo-mechanical devices. In this study, we designed pNIPAM microgel which is not only thermoresponsive but also capable of self-assembly with terpyridine (tpy) ligand-metal interaction to generate polymer nanostructures. We were able to control the size of microgel particles by varying the concentration of sodium dodecyl sulfate (SDS) in the reaction mixture, and the surface of pNIPAM microgel particles was functionalized with tpy. We confirmed that the resulting microgel particles can self-assemble in the presence of metal ions. Assembled nanostructures of tpy-pNIPAM microgels were characterized by scanning electron microscopy (SEM), dynamic light scattering (DLS) measurement and UV-Vis spectroscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-46**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

pH-Tunable Thermoresponsive PEO-based Functional Polymers with Pendant Amine Groups

이준희 김병수*

UNIST 화학과

Thermoresponsive polymers with high water-solubility exhibiting a lower critical solution temperature (LCST) in aqueous solution have attracted increasing attention for the development of smart biomedical materials. Herein, we report on the pH-tunable thermoresponsive poly(ethylene oxide) (PEO)-based functional polymers bearing pendant amine groups. Thermoresponsive polymers with pH-tunability are successfully synthesized by post-modification of the poly(ethylene oxide-co-allyl glycidyl ether) P(EO-co-AGE) copolymer using cysteamine, 2-(dimethylamino)ethanethiol, 2-(diethylamino)ethanethiol, 3-amino-1-propanethiol and 6-amino-1-hexanethiol. Well-defined, water soluble P(EO-co-AGE) copolymers are prepared via controlled anionic ring-opening copolymerization of ethylene oxide (EO) with 10 mol% of functional allyl glycidyl ether (AGE) comonomer. Respective aminoalkanethiols are introduced to side chains of P(EO-co-AGE) via a facile, modular thiol-ene click chemistry to provide a pH-tunable thermoresponsive property on the resulting copolymers. The LCST was determined by the transmission spectra of the 0.10 wt% aqueous polymer solutions under varying pH values. Depending on the parameters including the types of pendant amine groups, hydrophobicity of side chains and pH, the LCST value could be tuned from 44 to 100ºC. With their superior biocompatibility, this novel functional group chemistry will offer a new means to endow the pH-tunable thermoresponsive properties on the poly(ethylene oxide)s.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-47**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular interactions of thiourea-linked calix[4]arene and organophosphonate for nerve agent detection

김경수 이주현 조혜진 송창식*

성균관대학교 화학과

Calixarenes have been extensively used in various applications such as host-guest systems, molecular self-assembly, catalysis, membranes and non-linear optics. In this study, we have designed and synthesized thiourea-functionalized calix[4]arene (TC) of a cone conformation. To functionalize thiourea at the upper rim of calix[4]arene, we choose the condensation reaction of diaminocalix[4]arene with benzyl isothiocyanate. We were also able to prepare 1-benzyl-3-(4-propoxyphenyl) thiourea (BT) as a control using similar synthetic methods. The binding properties and molecular dynamics of synthesized TC and BT for dimethyl methylphosphonate (DMMP) were confirmed by nuclear magnetic resonance (NMR) spectroscopy. Substantial peak shifts were observed for TC in the position of thiourea moiety, which also appeared in BT. Interestingly, the peaks for calix[4]arene of TC were shifted simultaneously. We attributed this observation to the molecular dynamics of TC induced by DMMP, which was further supported by density functional theory (DFT) calculations. We also measured the binding capacity of TC and BT for DMMP by quartz crystal microbalance (QCM).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-48**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The First Cyclopolymerization of 1,6-Heptadiynes by Grubbs 1st Generation Catalyst

강철 최태림*

서울대학교 화학부

One of powerful ways to synthesize conjugated polymers is cyclopolymerization. Using olefin metathesis catalysts with diyne monomers, polyacetylene backbone can be easily constructed. Especially, cyclopolymerization of 1,6-heptadiynes give 5-membered rings bearing pi-conjugated system. And due to their planarity, the polymer have highly long effective conjugated length affording narrow band-gaps. Recently, our group developed living cyclopolymerization system using fast-initiating Grubbs catalyst with coordinating solvents or ligands. Meanwhile, there have been reports that side products are generated when cyclopolymerization is conducted with Grubbs catalysts. Our recent mechanistic studies have proven that this side reaction proceeds not by olefin metathesis process but by the action of decomposed Grubbs catalyst which mediates [2+2+2] alkyne trimerization. Especially, the side reaction was highly dominant when Grubbs first generation catalyst (G1), which is why the cyclopolymerization by G1 was never been reported. Herein, we report the first example of cyclopolymerization catalyzed by G1. By using acidic additives, we could successfully synthesize polymers with suppressing the generation of side products. Various monomers having different functional groups afforded polymers with moderate to good efficiencies. Through mechanistic studies, we concluded that the additive helps phosphine dissociation of Grubbs catalyst especially for conjugated Ru-carbene which is crucial for propagation. Also, it was confirmed that the additive prevents the deformation of propagating species and suppresses the [2+2+2] alkyne trimerization.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-49**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Regulating Sensing Property of Spiropyrans by Conjugation with Different Functional Groups via a Triazole Linkage

이주현 이민혜 최은정 송창식*

성균관대학교 화학과

Spiropyrans (SP) are well-known photochromic materials and they undergo cis-trans isomerization to a merocyanine (MC) by external stimuli such as UV/visible light, thermal energy, and metal ions. SP can be utilized to a colorimetric sensor because MC is showing a vivid color. Using “click chemistry”, we can induce functional groups easily. Cu-catalyzed alkyne-azide cycloaddition (CuAAC) is well-known as a click reaction since it is simple, fast, and has no side reaction. Triazole linkage that is formed by CuAAC can be utilized as a metal’s binding site and it may show selectivity for a number of metal cations. Our strategy is to change SP’s sensing and solvatochromic properties depending on different side groups. In this study, we compared the effects of different functional groups on the property of SP. The metal-ion sensing ability was measured by UV-vis spectroscopy, and ethylene glycol-functionalized SP (E-SP) showed more selective to Ca2+ than benzyl-functionalized SP (B-SP). Also, E-SP improved the water solubility and cyanide sensing ability, which was supported by UV-vis spectroscopy under aqueous environment. E-SP was applied to a paper sensor for cyanide because of its fast response and high intensity change in aqueous environment.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-50**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Disk-shaped Micro Particles by RAFT Polymerization

김태윤 정일두*

부산대학교 고분자공학과

Disk-shaped particles based on polycaprolactone (PCL) were synthesized using photodegradable polymethylvinylketone (PMVK) and used for drug delivery system. In this study, PCL based triblock copolymer was synthesized by RAFT polymerization and used to fabricate microsphere by emulsion-evaporation method. Disk-shaped particles were then prepared by UV-irradiation with the microsphere. In order to polymerize by RAFT method, PCL based macro-CTA (chain transfer agent) was first synthesized by reacting carboxylic acid-terminated CTA with PCL, and used for the synthesis of block copolymer with methyl vinyl ketone (MVK). The morphology of the particles before and after UV irradiation were confirmed by SEM and TEM images and the release behavior of paclitaxel, anti-cancer agent for female cancers, in disk shape particles were evaluated by HPLC. PCL based disk-shaped particles will be anticipated to enhance drug release and could find potential application for biomaterials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-51**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Dual Stumuli-Responsive Supermolecules

김태윤 정일두*

부산대학교 고분자공학과

Cyclodextrins(CDs) are a series of cyclic oligosaccharides consisting of 6-8 glucose units connected by α-1,4 linkages and used as drug delivery carriers to increase the aqueous solubility of poorly water-soluble drugs, and to increase their bioavailability and stability. Stimuli responsive polymers sensitive to external temperature, light or pH are of increasing interests because of their potential applications in biomedical field. In this work, stimuli responsive triblock copolymers were synthesized by the polymerization of n-isopropyl acrylamide(NIPAAm) by ATRP with pseudo polyrotaxane initiator, in which many β-CDs were threaded onto a poly(propylene glycol). Their lower critical solution temperatures (LCST) were determined by cloud point measurements over a range of pH environments. The structure of the resulting copolymers was characterized in various instruments

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-52**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Water-Soluble Fluorescent Probe for Mercuric(II) Ion Detection based on Chemical Reaction

이지애 정지은 우한영[1,*]

고려대학교 화학과 [1]고려대학교 이과대학 화학과

Mercuric ions, one of the most hazardous pollutants has been receiving much attention. Based on the binding affinity mercuric ions toward the ethyl mercaptan moiety, several fluorescent probe structures were designed to display high sensitivity and selectivity toward Hg2+. However, many previous Hg2+detection probes also response upon adding silver ions. Moreover, most mercuric ion detection was demonstrated in tetrahydrofuran (THF) or in a mixture of THF and water. It may decrease the binding affinity and the selectivity of the probe towards Hg2+ over other ions due to the poor solubility of Hg2+ ions in THF. Herein, we have studied water-soluble fluorescent Hg2+probes which show high sensitivity and selectivity based on the deprotection reaction of ethyl mercaptan. The detailed assay characteristics will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-53**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fracture toughness and ductile characteristics of diglycidyl ether of bisphenol-A resins modified with biodegradable epoxidized linseed oil

임윤지 박수진[*]

인하대학교 화학과

Epoxidized linseed oil (ELO) was synthesized to improve the biodegradability and fracture toughness of the diglycidyl ether of bisphenol-A (DGEBA). The ELO was characterized using Fourier transform infrared (FT-IR) spectroscopy, gel permeation chromatography (GPC), and epoxy equivalent weight (EEW) tests. DGEBA was blended with ELO contents from 10 to 40 wt% to obtain a modified network. DGEBA and the DGEBA/ELO blends were characterized by their biodegradability, thermal properties, and fracture toughness. The thermal properties of the DGEBA/ELO blends were investigated using differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The fracture toughness of the DGEBA/ELO blends was studied by measuring the Izod impact strength and the critical stress intensity factor (K_{IC}). The morphologies were observed by scanning electron microscopy (SEM). In the biodegradability results, the DGEBA/ELO blends degraded 5% of the initial weight. The thermal property results confirmed that the crosslinking density of the epoxy networks decreased. The impact strength of the DGEBA/ELO blends was significantly improved with the addition of ELO owing to the reduced cross-linking density of the epoxy network.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-54**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

EMI Shielding and Mechanical Properties of Multi-walled Carbon Nanotube-reinforced Biodegradable Epoxy Matrix Composites

임윤지 박수진*

인하대학교 화학과

Biodegradable epoxy (B-epoxy) was prepared from diglycidyl ether of bisphenol A (DGEBA) and epoxidized linseed oil (ELO). The mechanical properties of B-epoxy composites-reinforced with Multi-walled Carbon Nanotubes (MWCNTs/B-epoxy) were examined by dynamic mechanical analyzer (DMA), critical stress intensity factor (K_{IC}) tests, and impact strength tests. The electromagnetic interference shielding effectiveness (EMI-SE) of the composites was evaluated by means of the reflection and absorption methods. From the results, it was found that the mechanical properties of MWCNTs/B-epoxy were enhanced with increasing MWCNTs content, whereas the value decreased above 5 phr. MWCNTs content. This was probably considered that the MWCNTs entangled with each other in B-epoxy due to an excess of MWCNTs. The highest EMI-SE of the MWCNTs/B-epoxy composites was approximately 16 dB for 13 phr. at 1.4 GHz. The composites (13 phr.) met the minimum EMI-SE (90%) as shielding materials at 1.4 GHz. The EMI-SE of MWCNTs/B-epoxy was also increased with increasing MWCNTs content, which played a key factor to determine the EMI-SE.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-55**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study of cooperative binding of metal cations with triazole conjugated spiropyran-calix[4]arene

이민혜 이주현 정동철 송창식*

성균관대학교 화학과

We have synthesized spiropyran embedded Calix[4]arene conjugated with 1,2,3-triazole receptor for the recognition of series of metal cations Ca2+, Mg2+, Cd2+, Co2+, Fe2+, Hg2+, Ni2+, and Zn2+, in which mainly the lower rim of calix[4]arene has been modified. UV-vis absorption spectroscopic and naked-eye detection were used to differentiate the recognized metal cations. The receptor-cation binding mainly occurs through the combination of 1,2,3-triazole as well as methoxy and hydroxyl units at the open merocyanine form of spiropyran. The binding stoichiometry between receptors and metal cations were determined by various continuation method (Job's plot) and NMR studies. Interestingly, we found that cooperative binding mode for 1:2 binding ratio of receptor to metal cations. A cooperative binding effect was investigated by stepwise bindings of Mg2+ and BSP.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-56**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Porous PS nanoparticle by emulsion RAFT polymerization

장보윤 김태윤[1] 정일두[1,*]

부산대학교 화학공학.고분자공학과 [1]부산대학교 고분자공학과

Porous polystyrene(PS) particles were synthesized through surfactant-free emulsion polymerization in the ab initio batch condition based on RAFT(reversible addition-fragmentation chain transfer) polymerization. Water-soluble amphiphilic RAFT agent was synthesized from poly(ethylene glycol) methyl ether and 2-(dodecylthiocarbonothioylthio)-2-methylpropionic acid(DDMAT). Styrene was polymerized with methyl vinyl ketone(MVK) using ACPA as an initiator, and then it was photodegraded UV irradiation. PS particles were characterized with FT-IR(Fourier transform infrared spectroscopy), H-NMR. GPC and DLS confirmed the formation of narrow-distributed particles. Porous surface and morphology of particles were confirmed by SEM and TEM images. Porous PS particles are expected to be used in drug delivery system and future biomaterials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-57**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Nanoparticle based on DHPF polyurethanes for DNA delivery

강지인 박수용[1] 정일두[1,*]

부산대학교 화학공학,고분자공학과 [1]부산대학교 고분자공학과

DHPF(di-(2-hydroxypropyl) fumarate) has been developed for PPF(poly(propylene fumarate)) which is used for biodegradable scaffold. Here, we designed a biodegradable polyurethane(PFU) for delivery vehicle. PFU synthesized using DHPF, PEG(polyethylene glycol) and HDI(1.6-diisocyanatohexane) was designed to degrade through hydrolysis and enzymatic mechanisms due to its peptide bond in polymer backbond. For further experimental study, nanoparticles encapsulating complexes of DNA and linear polyethylenimine(LPEI) or bovine serum albumin labeled with fluorescein will be fabricated through water-in-oil-in-water emulsion. The nanoparticles are expected to have PEG on their surfaces which helps nanoparticles to avoid the immune system. The characteristics of these nanoparticles will be confirmed by TEM, DLS, cellular viability and confocal microscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-58**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electromagnetic Interference Shielding Effectiveness of Metal-plated MWCNTs/High-density Polyethylene Composites

임윤지 박수진[*]

인하대학교 화학과

Multi-walled carbon nanotubes (MWCNTs) were metal (Nickel)-plated chemically to enhance the electromagnetic interference shielding effectiveness (EMI-SE) of Ni-MWCNTs/High-density polyethylene composites (Ni-MWCNTs/HDPE). The surface properties of the Ni-MWCNTs were characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). The EMI-SE of the Ni-MWCNTs/HDPE was tested by a EMI shielding analyzer. The EMI-SE of 3-MWCNTs/HDPE and 3-MWCNTs (30-Ni) showed approximately 5 and 12 dB at 1.0 GHz, respectively. The EMI-SE of Ni-MWCNTs/HDPE was enhanced compared to that of as-received MWCNTs/HDPE. Our results indicate that the Ni-MWCNTs can lead to a EMI-SE improvement due to the EMI adsorption behavior of the nickel particles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-59**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of adamantane-based sp^3-rich carbon materials

CHEN XIONG 이선화 **Rodney Scott Ruoff**[1,*]

기초과학연구원 다차원탄소재료연구단 [1]UNIST 화학과

Diamond has been made by high-pressure high-temperature, chemical vapor deposition (hot wire CVD, PE-CVD), shock wave, using C_{60} as precursor, hydrothermal growth in metal-C-H_2O system, from silicon carbide, reduction-pyrolysis-catalysis synthesis, and laser pulse. Polymer with only sp^3 carbons can be converted by heating to diamond-like carbon. Adamantane, the simplest diamondoid molecules, is a ‘tricyclic saturated hydrocarbon’. It is a ten-carbon atom molecule that has the same spatial arrangement of carbon atoms in the diamond crystal. Adamantane-based compounds have been used to nucleate nanodiamonds on carbon nanotubes (CNTs). Here, we present a hyperbranched polymer with only saturated hydrocarbons using halogenated adamantane. Their synthesis and chain structure tuning will be presented. *This work was supported by IBS-R019-D1.*

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-60**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Characteristics of Polymer Solar Cells with Metal Oxide Nanoparticles

정재훈 서주역 김화정 김영규*

경북대학교 화학공학과

The performance of solution-processable polymer solar cells have been significantly improved by applications of new electron-donating conjugated polymers and/or novel non-fullerene electron-acceptors. Very recently, the power conversion efficiency of polymer:fullerene solar cells has reached ca. 11~13% by applying either single stack or tandem device structures. In addition to all-organic solar cells, hybrid solar cells have also attracted growing interest because of the benefits of inorganic materials in terms of stability and durability. Our group has been studying the addition of inorganic nanoparticles to the active layers of organic solar cells and reported a gradual improvement in stability by the presence of inorganic nanoparticles. In particular, considering the incompatibility between inorganic materials and organic materials, we have invented a couple of chemical modification technology for inorganic nanoparticles. This presentation demonstrates the basic approaches of polymer solar cells with chemically-modified inorganic nanoparticles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-61**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

내열성 및 내화학성이 우수한 Polysulfone공중합체 및 그 제조 방법

김미란 장윤주[1] 허성현[1] 임종관[1] 노형진[2,*] 권영도[3,*]

(주)삼양사 기능성소재PG [1](주)삼양사 화학연구소 [2]삼양그룹연구소 EP소재프로그램 [3]삼양사 화학 연구소 기능성 소재

Polysulfone 소재는 Super EP 로서 매우 우수한 기계적 특성과 화학적 특성을 지닌 소재이다. 최근 경량화 소재의 요구와 함께 가볍고 물성이 뛰어난 Polysulfone 의 사용처가 많이 늘어나는 추세이다. 또한 PSU 는 구조적인 특성상 RO 멤브레인의 지지체 및 MF, UF 중공사, 기체 분리막 소재 용도로도 많이 사용되고 있다. 그리고 삼양사에서 상업생산에 성공한 Isosorbide 는 식물 유래 물질로써 석유화학 모노머 대체로 친환경성을 가지며 지환족 구조상 내열특성이 있어 다양한 고분자에 코모노머로 사용된다. 뛰어난 물성을 가진 Polysulfone 에 식물유래 물질인 Isorbide 를 NMP 용매 베이스의 용액중합법으로 공중합 시켜 친환경성을 가지고, 내열성 및 내화학성을 더욱 향상시킨 Super EP 소재를 제조하고자 하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-62**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Control of Thermal property in Etheylene, Alkynes, and CO Terpolymer

임유나 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Polyketone has potential usage as industrial materials such as automotive, electronics due to excellent properties such as high impact strength, chemical resistance, etc. However, high melting polyketones required high temperature (above 250°C) for using as industrial materials. Moreover, polyketones have the thermal decomposition issue at 280°C. Therefore, to solve the problem of this issue, the development of new process is needed. In this study, new terpolymers was synthesized from ethylene, CO, and various aromatic alkyne as second olefin to achieve low melting polyketones. Through this study, we found that alkyne can be used as additional materials to control the thermal properties of polyketones.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-63**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structural Effect of Modified Thiourea-Based Receptors for Chemical Warfare Agent Detection by Quartz Crystal Microbalance

하성균 이민혜 조혜진 송창식*

성균관대학교 화학과

We have designed and synthesized thiourea-based receptors for gas-phase detection of dimethyl methylphosphonate (DMMP), a nerve agent simulant, using quartz crystal microbalance (QCM). QCM can detect very small mass-changes in real-time via reverse piezoelectric effect. The resonant frequency would shift by analyte adsorption/desorption at the surface of a quartz crystal and such shifts can be monitored by a counter through electrodes. We assumed that thiourea receptors could adsorb well DMMP molecules through hydrogen bonding with the organophosphonate moiety. In this study, we systematically designed and synthesized several thiourea receptors, and found in QCM measurement that the chemical structure of thiourea receptors greatly affect the sensing ability to DMMP. In order to get insight on the thiourea's structural effect, we investigated molecular interactions between thiourea receptor and DMMP by 1H-NMR spectroscopy. We also interpreted the sorption/desorption kinetics by Langmuir isotherm and thermodynamic data were compared.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-64**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

New Conjugated Donor-Acceptor Copolymer with pyrrolo-pyridazine containing metoxy-bithiophene Side Chain for organic thin film transistor

박규진 황도훈*

부산대학교 화학과

Two new polymers poly [6-(2-dodecylhexadecyl)-1-(5''-methyl-[2,2':5',2''-terthiophen]-5-yl)-4-(5-methylthiophen-2-yl)-5H-pyrrolo[3,4-d]pyridazine-5,7(6H)-dione](PPz-BT) and poly [1-(3'',4'-dimethoxy-5''-methyl-[2,2':5',2''-terthiophen]-5-yl)-6-(2-dodecylhexadecyl)-4-(5-methylthiophen-2-yl)-5H-pyrrolo[3,4-d]pyridazine-5,7(6H)-dione](PPz-MeOBT), which contained methoxy-substituted and non-methoxy-substituted bithiophene units respectively, were designed and synthesized. Introducing methoxy groups on the bithiophene units affected their optical, electrochemical and charge transport properties. Experimental results revealed that the introduction of methoxy group highered the HOMO and LUMO energy levels of polymers due to the electron donating ability of methoxy group. As a result, the maximum mobility of 4x10-3 cm2V-1s-1 was achieved in PPz-BT (at 280 ℃), while that of PPz-MeOBT was 4 x10-4 cm2V-1s-1 (at 280 ℃)..

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-65**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Telechelic Dianthraquinone Polybutadiene via ROMP and Study of Its Photo-Oxidation and UV Cross-Linking Behaviours

이정현 문봉진[1,*]

서강대학교 화학 [1]서강대학교 화학과

Polybutadiene is one of the most popular elastomers and installation of various functional groups on the chain ends has been extensively studied. Those telechelic polybutadienes can be obtained either by ring opening metathesis polymerization (ROMP) using a chain transfer agent or anionic polymerization. The polymers have been employed in the synthesis of various copolymers, gelation by chelation of end groups to metal ions, radical cross-linking reaction at polymer chain ends to enhance the mechanical strength, and etc.In this research, we prepared telechelic dianthraquinone-functionalized polybutadiene by ROMP and observed that the anthraquinone end groups act as sensitizing groups to induce photocrosslinking of the polymer. By introducing anthraquinone groups at the polymer chain ends, we could achieve homogeneous dispersion of the anthraquinone moieties in the polymer matrix, which is otherwise difficult due to the poor solubility and highly aggregating behavior of anthraquinones.The resulting polymer was irradiated under UV A (315 – 400 nm) for cross-linking and it was monitored by various experimental tools such as IR spectroscopy, rinsing and drying test, and UV-VIS spectroscopy. We found that the anthraquinone-functionalized polybutadiene was cross-linked in a short time of period (< 2 min) under UV irradiation, initiated by two anthraquinone end groups in every polymer chain. In addition, we could also observe photo-oxidation reaction of the polymer matrix during the UV irradiation.

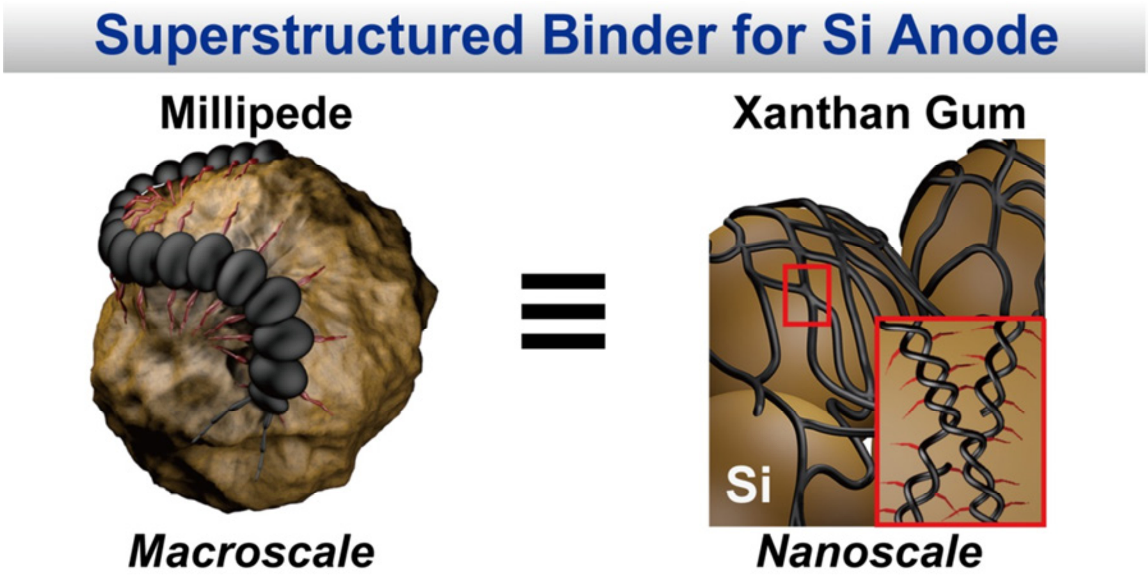
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-66**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Millipede-inspired structural design principle for high performance polysaccharide binders in silicon anodes

정유경 최장욱*

KAIST EEWS

It is widely accepted that polymeric binders play a critical role in the challenging cycling performance of silicon (Si) anodes in lithium ion batteries (LIBs). A variety of polysaccharides present in nature have shown good performance through many individual studies, but the comparison among them and molecular-level understanding of the critical parameters for their function within Si electrodes are presently unavailable. After a systematic study based on two standards, namely superstructure and electrostatic charge, xanthan gum turns out to perform better than any other polysaccharide as well as other classes of polymeric binders reported to date. Analogous to millipedes that exhibit extraordinarily strong adhesion onto versatile rough surfaces based on a continuous series of legs and micron-sized adhesive pads, the superior performance of xanthan gum can be explained by its double helical superstructure with a series of trisaccharide side chains and ion–dipole interactions from the charged functional groups. The current investigation suggests a general principle for the Si binder design that the superstructure and presence/position of charge interactions are the most critical parameters for stable cycling, which would certainly help the community to identify better natural binders in the future.(Ref. Energy Environ. Sci. 2015, 8, 1224)Keywords: polymeric binder; polysaccharide; superstructure; silicon anodes; lithium ion battery


Superstructured Binder for Si Anode
Millipede
Xanthan Gum
≡
Si
Macroscale
Nanoscale

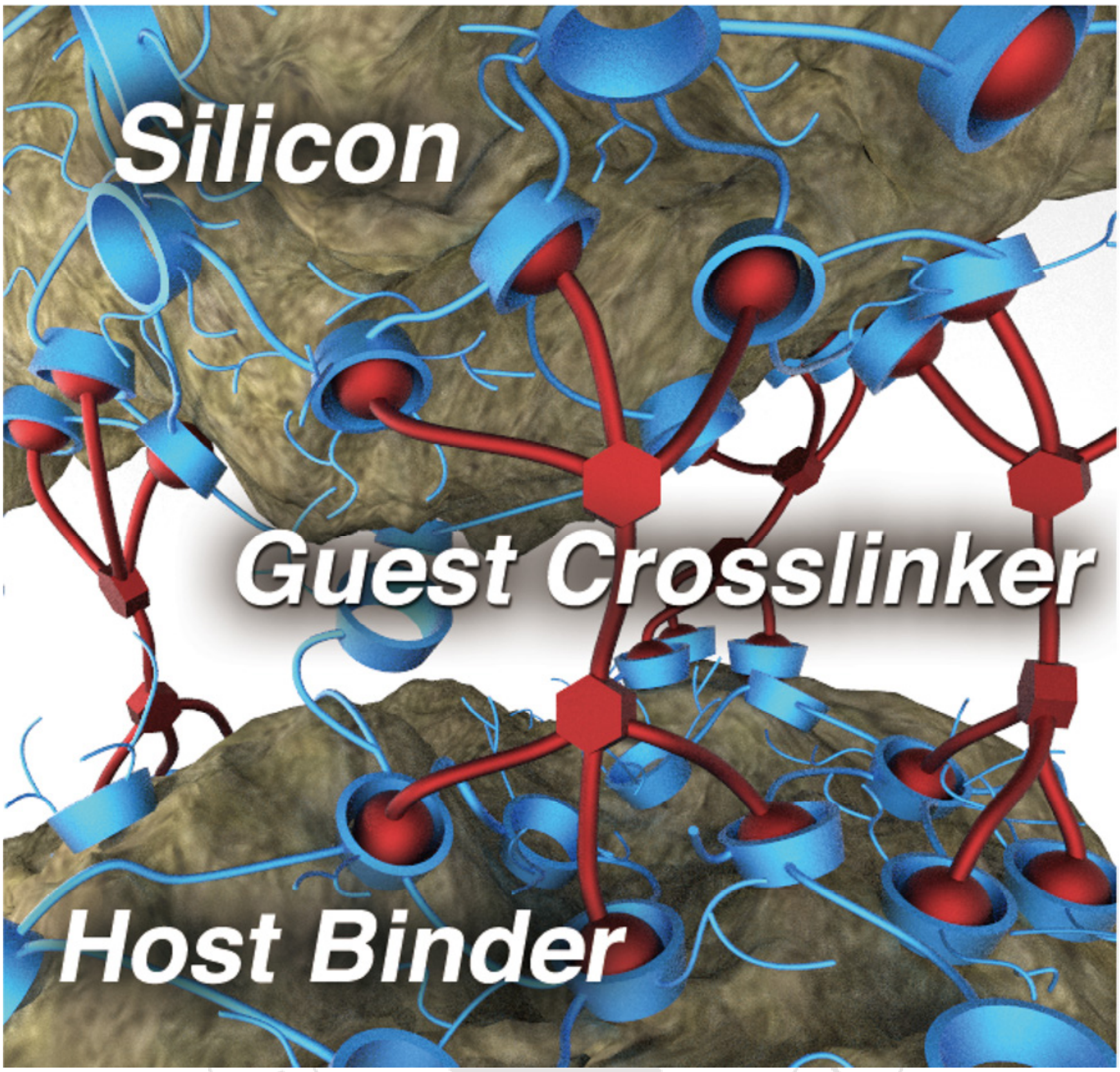
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-67**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dynamic Cross-Linking of Polymeric Binders Based on Host–Guest Interactions for Silicon Anodes in Lithium Ion Batteries

정유경 최장욱*

KAIST EEWS

We report supramolecular cross-linking of polymer binders via dynamic host–guest interactions between hyperbranched β-cyclodextrin polymer and a dendritic gallic acid cross-linker incorporating six adamantane units for high-capacity silicon anodes. Calorimetric analysis in the solution phase indicates that the given host–guest complexation is a highly spontaneous and enthalpically driven process. These findings are further verified by carrying out gelation experiments in both aqueous and organic media. The dynamic cross-linking process enables intimate silicon–binder interaction, structural stability of electrode film, and controlled electrode–electrolyte interface, yielding enhanced cycling performance. Control experiments using both α, γ-CDp with different cavity sizes and a guest molecule incorporating a single adamantane unit verified that the enhanced cycle life originates from the host–guest interaction between β-cyclodextrin and adamantane. The impact of the dynamic cross-linking is maximized at an optimal stoichiometry between the two components. Importantly, the present investigation proves that the molecular-level tuning of the host–guest interactions can be translated directly to the cycling performance of silicon anodes. (Ref. ACS Nano 2015, 9, 11317)Keywords: polymeric binder; dynamic cross-linking; host−guest interaction; silicon anodes; supramolecular chemistry, lithium ion battery


Silicon
Guest Crosslinker
Host Binder

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-68**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation and Characterizations of Copolycarbonates based on Bio-based Isosorbide and 1,4-Cyclohexanedimethanol

박슬아 최재훈 황성연* 오동엽* 박제영*

한국화학연구원 바이오화학연구센터

A series of copolycarbonates were synthesized by melt polycondensation of isosorbide (ISB), 1,4-cyclohexanedimethanol (CHDM), and diphenyl carbonate (DPC). The rigid structure of ISB affects increasing melt viscosity, which resulted in lower degree of polymerization. In order to overcome this difficulty, cationic additives were incorporated into the reaction as catalysts and surfactants, as well. Interestingly, the addition of cationic additives was also effective in improving mechanical properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-69**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

전기방사를 이용한 아가로스 나노섬유 제작 및 세포 배양

김민정 홍상은 장경주 윤국로*

한남대학교 화학과

아가로스는 홍조류로부터 추출하여 겔(gel)화하는 특성을 가진 천연 다당류의 일종이다. 생체적합성이 뛰어난 아가로스는 식품, 화장품, 제약, 생의학 등의 넓은 분야에서 응용되고 있다. 본 연구에서는 전기방사를 이용하여 아가로스 나노섬유를 제작하였다. 제작된 아가로스 나노섬유는 스케폴드(Scaffold)로서 조직 공학적으로 응용하기 위해 섬유아세포를 배양하고 나노섬유에서의 cell viability 을 확인하였다. 나노섬유의 물리적 특성은 광학현미경 (OM), 주사현미경 (SEM), 적외선분광기 (FT-IR), 접촉각 (contact angle), 열 중량분석기 (TGA), 인장응력 (Tension stress-strain)로 확인하였고 나노섬유에 배양한 섬유아세포는 공초점 레이저 주사현미경 (CLSM)과 주사현미경 (SEM)을 이용하여 확인하였다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-70**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of functionalized multi-layer nanofibers using biomaterials

장경주 홍상은 윤국로*

한남대학교 화학과

The biomedical and cosmeceutical applications of electrospun fibers remain the most interesting research field. Nanofibers can contribute in diverse emerging medical and cosmeceutical areas such as drug delivery, organogenesis, genomic medicine, rapid bedside clinical tests, smart wound dressings and mask pack. Multi-layered nanofibers were prepared by electrospinning of different layers using layer by layer and mixed spining. The resulting multi-layered nanofibers were characterized by OM (Optical microscopy), FE-SEM (Field Emission Scanning electron microscopy), FT-IR (Fourier Transform Infrared Spectroscopy), Contact angle, UTS (Ultimate Tensile Strength), TGA (Thermogravimetric Analysis), ^{1}H-NMR (^{1}H Nuclear Magnetic Resonance) and UV-VIS (Ultraviolet-Visible Spectrophotometer). These results of Multi-layered nanofiber were expected for the potential application of medical and cosmetic material.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-71**

발표분야: 고분자화학

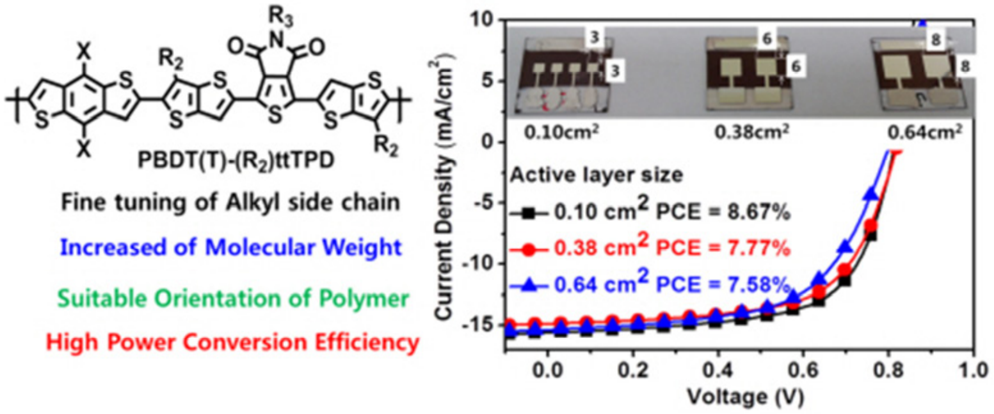
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of Thieno[3,4-c]pyrrole-4,6-(5H)-dione Based Conjugated Polymer Side Chains for High-Performance Organic Photovoltaic Cells

이성림 박종백 황도훈*

부산대학교 화학과

Optimization and analysis of conjugated polymer side chains for high performance organic photovoltaic cells (OPVs) reveal a critical relationship between the chemical structure of the side chains and photovoltaic properties of polymer-based bulk heterojunction OPVs. In particular, the impact of the alkyl side chain length on the π-bridging (thienothiophene, TT) unit is considered by designing and synthesizing a series of benzodithiophene derivatives (BDT(T)) and thieno[3,2-b]thiophene-π-bridged thieno[3,4-c] pyrrole-4,6(5H)-dione (ttTPD) alternating copolymers, PBDT(T)-(R_2)ttTPD, with alkyl chains of varying length on the TT unit. Using a combination of 2D X-ray diffraction, Raman spectroscopy, and electrical device characterization, it is elucidated in detail how these subtle changes to the chemical structure affect the molecular conformation, thin film molecular packing, blend film morphology, optoelectronic properties, and hence overall photovoltaic performance. For copolymers employing both the alkoxy or alkylthienyl-substituted BDT motifs, it is found that octyl side chains on TT unit yield the maximum degree of molecular backbone coplanarity and result in the highest quality of molecular packing and optimized hole mobility. Inverted devices fabricated using this PBDTT-8ttTPD: polymer/[6,6]-phenyl-C_{71}-butylic acid methyl ester active layer show a maximum power conversion efficiency (PCE) of 8.7% with large area cells (0.64 cm^2) maintaining a PCE of 7.5%.


X
R$_2$
R$_3$
O
N
O
S
S
S
S
S
R$_2$
X
PBDT(T)-(R$_2$)ttTPD
Fine tuning of Alkyl side chain
Increased of Molecular Weight
Suitable Orientation of Polymer
High Power Conversion Efficiency
Current Density (mA/cm^2)
10
5
0
-5
-10
-15
0.0
0.2
0.4
0.6
0.8
1.0
Voltage (V)
3
3
6
6
8
8
0.10cm^2
0.38cm^2
0.64cm^2
Active layer size
0.10 cm^2 PCE = 8.67%
0.38 cm^2 PCE = 7.77%
0.64 cm^2 PCE = 7.58%

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-72**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The influence of alkyl chain containing silanes on the hardness and flexibility of silicon based organic-inorganic hybrid materials

박제승 문봉진*

서강대학교 화학과

Recently, flexible displays are emerging as the next generation display. The most significant features of flexible display include its foldability and/or rollability. In this sense, highly required is a new material that can replace the glass window with high flexibility maintaining the comparable hardness of glass. Among many other candidates, polysilsesquioxane type organic-inorganic hybrid materials have drawn much attention in this area. Polysilsesquioxanes(PSQs) that comprise a class of organic-inorganic hybrid materials can be classified into the following three structures.1) Random branched sols2) Polyhedral oligomeric silsesquioxanes(POSS)3) Ladder-like polysilsesquioxanes(LPSQ)In these three structures, only POSS and LPSQ can be uniformly characterized to be of controlled structures. POSS generally possess oligomeric three-dimensional cage structures while a hypothetical LPSQ is a polymeric analogue with a linear, double-strained siloxane backbone. Especially, LPSQ is reported that superior thermal stability, solubility, and improved film properties. So, we judged that LPSQ is more suitable for flexible display hard-coating materials. We designed and synthesized a new LPSQ and investigated the structure-property relationship by changing the ratio of alkyl group containing flexible monomers. Introduction of flexible substituent was expected to enhance the flexibility to make some space in the LPSQ structure. By the experiment changing the ratio of the flexible substituent, we could investigate the correlation between flexible substituent and flexibility/hardness. References1. Choi, S.S.; Lee, A.S.; Hwang, S.S.; Beak, K.Y. Marcromolecules, 2015, 48, 6063-6070

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-73**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cell Surface Engineering with Antimicrobial Chitosan Shell

김범진 최인성*

KAIST 화학과

Cell surface engineering is defined as a chemical methodology aimed to functionalize or modify the surface of individual cells by encapsulating them within nano-thick artificial shell. By modifying cell surfaces, it is possible to control interactions between cells and the external environment as well as manipulate cell properties. The cell encapsulation for cell surface engineering has mainly been executed through the layer-by-layer (LbL) deposition technique based on the electrostatic interactions or hydrogen bonding, and various cells ranging from microorganisms to human cells have been modified with various types of nanomaterials, such as polymers, nanoparticles, nanotubes, and graphene oxide.Cytocompatibility of the materials is an essential precondition for cell surface engineering, because the cells have to be exposed to the materials of artificial shell during the cell encapsulation. So it imposes a constraint on the use of a wider range of materials in cell surface engineering. In addition, sometimes, the valuable materials, used for functionalization of microbial surface that are found to be cytocompatible, demonstrate their toxicity when applied to that of mammalian cells. For these reasons, material-independent cell encapsulation is required for more diverse cell surface engineering. In this work, we developed a simple method for material-independent cell surface engineering. By pre-depositing the cytocompatible multilayers on the cell surface, the chitosan(CTS), a representative antimicrobial material, could be used as the component of artificial shell on the cell surface without loss of encapsulated cell viability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-74**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Charge-Dependent Cellular Uptake of Spherical Polymeric Nanoparticles

황주영 곽민석*

부경대학교 화학과

Passive targeting is a strategy toward personalized medicine and cancer nanotherapy, where nano-sized delivery vehicles do not have any ligand for receptor-mediated endocytosis. In passive targeting, several parameters such as size, shape and charge govern the effectiveness of cellular uptake. Here, we present a method to control the density of charges on surface of nanoparticles(NPs). We prepared fluorescent NPs(d = 10 nm) covered with 0 – 100 % positive and negative charges in every 10% interval and characterized the NPs by dynamic light scattering, zeta potential and gel electrophoresis. Then passive cellular uptake in fourteen cell lines using the NPs was investigated by fluorescence microscopy. We found out that, three cell lines exhibit specific charge-dependent uptake, which also agree to flow cytometry. These findings may contribute to understand fundamental role of charges on NPs for applications in therapeutics and diagnostics.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-75**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Charge- and Shape-Specific Cellular Uptake of Au Colloids and Application in Photothermal Cancer Therapy

김미진 곽민석*

부경대학교 화학과

Charged nanovehicles in different shapes can target human cancer cells with high affinity and specificity. This passive targeting can be tuned either by the specific charge and coverage on the surface or by shape. First, we synthesized two lipoic acid derivatives with negatively and positively charged functional groups, sulfate and trimethylammonium chloride, respectively. Via S-Au bond, charge can be introduced on the surface of Au colloids such as spherical nanoparticles (NPs) and nanorods (NRs). To a human cervical cancer cell line, HeLa, we fed positively or negatively charged Au colloids to passively target the cells to study the effect of charge and shape in passive cell uptake. Since near-infrared irradiation to NRs can induce heat, we further applied the materials to photothermal therapy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-76**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Rylene Dye-Loaded Probe Nanoparticles for Visible-Infrared Imaging

강민경 Chen Li[1] Klaus Muellen[1] 곽민석*

부경대학교 화학과 [1]Max-Planck-Institute for Polymer Research, Germany

Rylene dyes exhibit superior photophysical properties including outstanding chemical and photochemical stabilities as well as high fluorescence quantum yields (FQYs). However, the rylene chromophores are highly hydrophobic to use them as molecular probes. We present a general incorporation method to load the molecules within micelle core of triblock copolymer and stabilize the core. The presence of rylene dyes in confined hydrophobic environment fairly preserve their FQYs in aqueous media. Twenty one probe nanoparticles (PNPs) loaded with rylene dyes, in the spectral region of visible and infrared (400 – 750 nm) were prepared and their photophysical properties were characterized. The PNPs may pave the way for a new class of fluorescence probes applicable in in vitro and in vivo imaging.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-77**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Active vs Passive Targeting: Preparation and Cellular Uptake of Nanoparticles with Folic Acid and/or Charges

김해주 곽민석*

부경대학교 화학과

We investigated effect of passive and active ligands in cellular uptake. First, both hydroxyl termini of PEO-b-PPO-b-PEO were converted to folic acid(FA; ligand) and trimethylammonium bromide(AB; charge). Then micelle core of FA and AB polymer blends was stabilized by semi-interpenetrating network formation in the presence of fluorescent probe, Nile Red. Lastly, cellular uptake of nanoparticles varying charge and ligand was studied in HeLa by fluorescence microscopy and flow cytometry.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-78**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solution-floating method for simultaneously inducement of self-assembly and thin film generation of P3HT on water substrate

김용재 전환진[1,*]

KAIST 생명화학공학과 [1]KAIST 나노종합기술원

Conventional processing of well-made conjugated polymer film for organic electronics has some limitations. To achieve efficient method, the single step fabrication of conjugated polymer thin film have been required because self-assembly inducement of conjugated polymer and thin film fabrication process are essential for thin film devices. Here, we introduce solution-floating method, a highly efficient method for fabricating uniform, large-area semiconducting thin films composed of poly(3-hexyl thiophene) (P3HT) nanowires (NWs) During the evaporation of the floated organic solvent, well-dissolved P3HT chains are self-assembled into one-dimensional P3HT NWs, and these NWs then form a thin film. Systematic TEM experiment presents for the first time the unique self-assembly mechanism behind the formation of P3HT NWs from the self-assembly of P3HT micelles. Also, the properties of good solvent such as solubilities in water and evaporation rate affect nanomorphologies of thin films formed by solution-floating method. The floated P3HT NWs thin film on water can be easily transferred onto a Si wafer, bestowing advantages for the fabrication of a high-performance organic field-effect transistor (OFET) device with an excellent carrier mobility of 0.012 cm2/V·s.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-79**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and properties of polyurethane / acrylate hybrid aqueous emulsions using a surfactant free method

구동명

인하대학교 고분자공학과

In this study, we have prepared core-shell type acrylic polyurethane hybrid emulsions containing reactive groups by surfacntant free polymerization method. In this emulsion, the shell part is composed of polyurethane polymers containing pendant carboxylicgroups and vinyl end groups and the core part is composed of acrylic copolymer. Also, mechanical strength properties, average particle size, reation and storage stability of the polyurethane acrylate hybrid emulsion were studied and compared with waterborne polyurethane content. To improve water resistance of dried hybrid emulsion, we adjusted controlled waterborne polyurethane and emulsion content respectively

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-80**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preperation and themomechanical properties of polyurethane-based shape memory polymer

구자민

한국외국어대학교 화학과

This study is to investigate the thermomechanical properties of polyurethane-based shape memory polymer according to the change of hard-soft segment moral ratio. SMPs were prepared two different methods, one is solution polymerization using 4,4'-methylenediphenyl diisocyanate(4,4-MDI), polycaprolactone diol(PCL, Mn= 1000, 2000), polycarbonate diol(PCD, Mn= 1000, 2000), 1,4-butane diol(1,4-BD) and dimethylformamide(DMF). Another is bulk polymerization method using multifunctional isocyanate and polyether polyol. the prepared SMPs were characterized by differential scanning calorimetry(DSC) and dynamic mechanical analysis(DMA).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-81**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Folding of 2D structures into a 3D structure from a bilayer of photothermal conducting polymers

임한휘 김은경*

연세대학교 화공생명공학과

The conversion of photons to heat in the conductive polymer films causes local heating to increase temperature at the light exposed area. The resultant heat can be converted into other type of energy such as electrical, mechanical, or chemical energy. In particular the photothermal energy conversion into mechanical energy gives a unique method for reversible change from 2 dimensional to 3 dimensional structure on command. Herein we present a bilayer film prepared from conjugated polymers which was transferred onto a soft polymeric film, to form a bimorph. The resultant 2D structures was reversibly folded into a 3D structure through photothermal stimuli, to afford biomimetic complex 3D structure. Effect of the chemical structure and composition in the bimorph on the sensitivity of structural conversion will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-82**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

다양한 아민으로 중화된 술포네이트 폴리스타이렌 아이오노머의 열에 의한 상처 치유

조명근 유정아[1,*] 김준섭[2,*]

조선대학교 응용화학소재공학과 [1]조선대학교 화학교육과 [2]조선대학교 생명화학고분자공학과

본 연구에서는 다양한 아민으로 중화된 술포네이트 폴리스타이렌 아이오노머의 표면 상처가 열에 의해 어떻게 치유되는지를 조사하였다. 상처가 있는 아이오노머 시료를 열처리하여 치유 정도를 측정한 결과를 중화가 안 된 산 작용기를 가진 공중합체 시료와 알칼리 금속인 Na 로 중화된 아이오노머 시료가 보여 주는 치유 정도와 비교하였다. 아민으로 중화된 경우에는 산 작용기를 가진 공중합체나 Na 로 중화된 아이오노머의 경우 보다 상처 치유가 열처리에 더 민감하다는 것을 알 수 있었다. 이런 결과가 나온 이유는 크기가 큰 아민을 중화제로 사용한 경우에 그 아민 화합물이 중화제인 동시에 이온 회합체 가소제로 작용하기 때문에 이 두 요소가 상처 치유 정도에 반대로 영향을 미치기 때문인 것 같다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-83**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of wood adhesives based on carbohydrates and pMDIs

이향렬

한국교통대학교 생명공학과

To investigate the adhesion effect of various kinds and contents of polymeric methylene diphenyl diisocyanates (pMDIs) on adhesion performance, wood adhesives (A-1 ~ 5) were synthesized and characterized. As results, when the amount of pMDI increased in adhesives, the dry tensile strength was found to be proportionally increased sustaining at around 16.0 ~ 21.6 kgf/cm2. The polyurethane (PU) resin, which used M11S as a source of pMDI showed the best wet tensile strength at 11.9 kgf/cm2 and cyclic boil tensile strength at 8.1 kgf/cm2, which satisfied the requirement of over 7 kgf/cm2. This was supported by Korea National University of Transportation in 2016.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-84**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Thermal properties of wood adhesives based on carbohydrates and pMDIs

이향렬

한국교통대학교 생명공학과

The use of formaldehyde based adhesives such as urea-formaldehyde(UF) and phenol-formaldehyde(PF) have recently drown the attention of the public due to environmental issue. Formaldehyde can be produced by decompositions and will gradually release to the surrounding environment. We have developed a procedure to synthesize environment-friendly carbohydrate-pMDI based wood adhesives and investigated their physical properties. Thermal properties of the rice powder (RP) based polyurethane resins were characterized by differential scanning calorimetry (DSC) and Thermal gravimetric analysis (TGA). Thermal stability of polyurethane resins increased to 250℃ with adding pMDIs. The more pMDI (M5S) was added to adhesive, the higher thermal stability of the resin was observed by TGA. Tc of the resin (RP:M5S=1:3) showed at 107.3℃, whereas the resin (RP/M20S = 1:3) showed much lower Tc at 99.6℃. Thermal stability of PU resins increased to 250℃ with adding pMDIs. The more pMDI(M5S) was added to adhesive, the higher thermal stability of the resin was observed by TGA. This was supported by Korea National University of Transportation in 2016.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-85**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Dual responsive hydrogel microfibers fabricated by using microfluidic device

김동완 윤진환*

동아대학교 화학과

We developed the preparation method for the hydrogel microfibers and microtubes with acrylate monomers by using the microfluidic devices and alginate templates. Based on our development, we fabricated the hydrogel microfibers comprising poly(*N*-isopropylacrylamide) (PNIPAm) based copolymers incorporating amine or acrylate function groups for pH responsiveness. We found that the size of the microfibers can be controlled by the pH of the medium, which was induced by protonation or deprotonation of the pendant groups. Also, we confirmed the thermal responsiveness of prepared PNIPAm based microfibers with measurement of diameter changes in each pH solution and temperature. We expect that the dual responsive microfibers can represent the attractive scaffolds for tissue engineering and biocompatible applications

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-86**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

다양한 양이온으로 중화한 PEA 아이오노머의 열에 의한 치유 거동

소인섭 유정아[1,*] 김준섭[2,*]

조선대학교 신재생에너지융합학과 [1]조선대학교 화학교육과 [2]조선대학교 생명화학고분자공학과

다양한 양이온(소듐, 세슘, 바륨, 및 아연)으로 부분중화된 PEA 아이오노머의 기계적인 특성을 연구하였다. 그 결과, 산 작용기의 함량이 10.7 mol%인 PEA-Na 아이오노머는 중화도가 증가함에 따라 치유 효과가 커져 아이오노머의 항복 강도와 영 모듈러스가 증가하였다. 또한, 열 처리 시간이 1 시간에서 12 시간으로 증가함에 따라, 시편의 연신율이 증가함을 관찰할 수 있었다. 특히, 낮은 이온기 함량의 시편에서 더 높은 연신율이 관찰되었다. 한편, 이온기의 함량이 같을 때에는, 중화한 양이온의 종류가 아이오노머의 항복 강도와 영 모듈러스에 중요한 영향을 끼쳤다. 항복 강도를 살펴보면 소듐으로 중화한 아이오노머가 가장 높은 값을 보여 준다. 반면에, 바륨으로 중화한 아이오노머는 가장 낮은 값을 보여주었다. 또한, 아이오노머의 영스 모듈러스는 Na > Ba > Cs > Zn 순서로 증가하였다. 이러한 결과로부터, 아이오노머 이온 회합체 안의 이온쌍 사이에 작용하는 힘이 아이오노머의 치유 거동에 중요한 역할을 하는 것을 알 수 있었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-87**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Stepwise switching of thermotropic glazing comprising multi-component copolymers of gradient monomer compositions

이은수 김도완 윤진환*

동아대학교 화학과

Glazing for solar control is the most promising for energy efficient development. The switching mechanism of thermotropic glazing is dominated by the temperature-induced aggregation of the materials in the solvent above the lower critical solution temperature (LCST). An important constraining factor for the practical application of thermotropic glazing is the inability to control the transmittance in a stepwise manner on demand. To control the transmittance in a stepwise, LCST behavior of thermotropic polymers need to have wide temperature range. In this work, we have developed synthesis method to prepare multi-segmented copolymers that each segment having different compositions of the monomers. The obtained copolymer exhibits a volume phase transition over a wide temperature range, that is different from random or block copolymers. Solar control glazing was fabricated with multi-segmented copolymer, enabling stepwise solar control as well as visibility control.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-88**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Programmable volume phase transition of hydrogels for static motion bilayer actuators with large thermal hysteresis

김도완 이은수 윤진환*

동아대학교 화학과

Programmable volume phase transition of the hydrogel was achieved by the large thermal hysteresis of poly(*N*-isopropylacrylamide)-*graft*-methylcellulose hydrogel (PNIPAm- *g*-MC), which was prepared through the grafting of PNIPAm onto a MC backbone and simultaneous crosslinking of the chains. Due to the stabilized aggregates formed by the intermolecular interactions of the MC backbone, a large thermal hysteresis in volume change could be achieved. By combining the prepared hydrogel with photothermal materials, programmable volume change can be triggered by light irradiation and excessive cooling. We demonstrated that static bending of the fabricated bilayer actuator that comprising PNIPAm-*g*-MC/MNP as the active layer and PAAm as the passive layer in response to light irradiation is possible, meaning that the material has the ability to memorize its irradiation history, and have that memory erased by cooling.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-89**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation of Clustered Metal Nanoparticles from PS-PAA micelles Containing Au Nanoparticles

Zakia Maulida 제남진 유성일[1,*]

부경대학교 화학융합공학 [1]부경대학교 고분자공학과

In a selective solvent, diblock copolymers self-associated into spherical micelles consisting of soluble coronas and insoluble cores. Owing to the chemically distinct core and corona structures, micelles have been widely utilized as stabilizing agents for many functional materials. In particular, metal, semiconductor, and oxide nanoparticles have been encapsulated into the core of micelles for various applications. In this study, we first prepared PS-PAA micelles encapsulating Au nanoparticles in the core, which has been utilized as building block for the second-level assembling process. By controlling several experimental parameters such as temperature, solvent, and salt concentration, we could induce the re-organization of PS-PAA micelles into a larger micellar assemblies, at which multiple clustered NPs are positioned at the center of the assemblies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-90**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

PS-PAA 마이셀을 활용한 코어-코로나 이종 나노입자 합성

제남진 Zakia Maulida 유성일[1,*]

부경대학교 화학융합공학 [1]부경대학교 고분자공학과

블록공중합체는 선택적 용매에서 코로나 블록과 코어 블록으로 이루어진 구형의 마이셀을 형성한다. 본 연구에서는 polystyrene-block-poly(acrylic acid), PS-PAA, 블록 공중합체가 형성하는 마이셀을 이종의 나노입자로 기능화 시키고 이를 모델 촉매 반응에 적용하는 연구를 진행하였다. 이에, 마이셀의 코어에는 금 나노입자를 도입하고 코로나에는 은 나노입자를 합성하여 서로 다른 나노입자를 동시에 함유하는 마이셀 나노구조체를 제조하였다. 형성된 마이셀 기반 나노구조체는 광열전환 특성과 촉매반응의 활성화 에너지를 조절하는 특성을 나타내었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-91**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

MDD 기술을 이용한 M13 바이러스 기반의 새로운 계층적 나노 구조체 개발

한지예 김인홍[1] 오진우[2,*]

부산대학교 나노융합기술 [1]부산대학교 에너지융합연구소 [2]부산대학교 나노소재공학과

최근 물리, 화학, 재료, 전자, 생명공학 등 다양한 분야에서 생체 친화적 물질을 활용한 연구 및 소자의 개발이 각광을 받고 있다. 특히, 바이오 물질이 가지는 자가조립에 의한 정렬 특성을 이용하여, 바이오센서, 태양전지, 이차전지, 메모리 소자 등의 기능성 나노 구조체의 개발에 대한 연구가 활발히 진행되고 있다.자가조립을 이용한 기능성 나노 소자의 제작은 기존의 리소그래피 공정이 가지는 복잡한 나노 구조 및 대면적 패터닝의 어려움, 고비용 등의 단점을 보완하고, 간단한 공정과정을 통해 정교한 패턴과 계층적 나노 구조의 개발을 가능하게 한다. 이에 본 연구에서는 생체 친화적 물질이며, 일정한 크기 및 형태를 가지는 M13 바이러스를 이용하여 새로운 계층적 나노 구조체를 제작하였다. 이를 위해, 다양한 필름 제작에 일반적으로 사용되는 MDD 공정을 통한 자기조립 기법에 바이러스를 접목하여, 새로운 계층적 구조체 기반의 필름을 제작하였다. 제작된 바이러스 필름에 대해 AFM 을 이용하여 표면 구조 및 패턴을 분석하였고, 바이러스 입자의 농도, 용액 내의 확산 정도, 전기적 특성, 코팅 속도 등을 고려하여 계층적 나노 구조의 생성 원리에 대해 연구하였다. 또한, 적층 기술을 이용하여 바이러스 필름의 이온 필터 활용 가능성에 대해 연구하였다.본 연구에서 제작된 바이러스 필름은 기존의 바이러스 나노 구조체에서 발견되는 다발형태의 구조 외에, 줄무늬 패턴과 다공성 구조 등 새로운 나노 구조를 보였다. 이러한 특이적 구조는 바이러스의 농도와 코팅 속도에 의존하며, 용액 내 바이러스의 확산 정도에 직접적인 연관성을 가졌다. 바이러스 필름을 이용해 제작된 필터는 나트륨 및 염소 이온에 대해 우수한 선택적 검출 특성을 나타내어, 생체 친화적 물질 기반 이온 센서로의 활용 가능성을 보여주었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-92**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of poly(β-peptide) with controlled stereochemistry and molecular weight

정록암 이희승*

KAIST 화학과

Nature exhibits an abundance of structural materials in the form of protein fibers, which have attained remarkable levels of efficiency and performance through evolutionary selection. Protein fibers such as silk are composed of polyamide, silk is also the strongest natural fiber known.[1] Nylon 3-polymer characteristics are similar to silk and it is known to have bioactivity.[2] But this nylon 3-polymer can be synthesized in the form of chain or cis only.[3]In this study, Efficient synthesis of stereochemistry and molecular weight controlled poly(β-peptide) carried on. We selected a chiral β-amino acid (S,S)-trans-2-aminocyclopentanecarboxylic acid(ACPC), which is an amino acid with a rigid cyclopentane ring. A chiral monomer was synthesized and then a chiral polyamide was formed through polymer reaction in solution. Then, this chiral polyamide polymer's characteristics were analyzed. This study will consider a characteristics of synthesizing peptides, which have excellent biocompatibility for high molecular weight from chirality controlled β-amino acid and analyze their structures including helical structure and physical characteristicsReferences1. G. Q. Xu, L. Gong, Z. Yang and X. Y. Liu, Soft Matter, 2014, 10, 2116. 2. B. M. Mowery, A. M. Lindner, B. Weisblum, S. S. Stahl and S. H. Gellman J. Am. Chem. Soc. 2009, 131, 9735.3. Zhang, J. H.; Kissounko, D. A.; Lee, S. E.; Gellman, S. H.; Stahl, S. S. J. Am. Chem. Soc. 2009, 131, 1589

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-93**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Study of Environmental-friendly Non-crosslinked Polypropylene Having Excellent Thermal Stability and Electrical Properties for Power Cable Insulation

장상미 문병철[1,*]

일진전기 전선기술연구소 [1]일진전기 전선기술연구소

Cross-linked polyethylene (XLPE) is generally used for insulation material in power cable. However XLPE has environmental problem due to use of crosslinking agent and thermal stability of XLPE is insufficient for high temperature power cable operating at 110℃To increase electric power supply and develop environmental-friendly power cable, we need the development of new insulation material having excellent thermal properties without using crosslinking agent for alternative of XLPE. In this study, we prepared thermoplastic olefin (TPO) based polypropylene (PP) having higher melting temperature than XLPE as insulation materials. And we conducted the evaluation of thermal, mechanical and electric properties.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **POLY.P-94**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

M13 박테리오파지 기반의 메탈 나노와이어 합성 및 응용

안정태 김인홍[1] 오진우[2,*]

부산대학교 차세대기판학과 [1]부산대학교 에너지융합연구소 [2]부산대학교 나노소재공학과

최근 물리, 화학, 전자, 바이오 등 다양한 분야에서 나노 구조가 가지는 우수한 전기, 화학적 물성 및 구조적 특성을 이용한 새로운 기능성 소재의 개발에 대한 연구가 많은 관심을 받고 있다. 특히, 전자기기의 소형화에 따른 핵심 소자의 개발, 에너지 변환 및 저장을 위한 광·전자 소자의 개발 등에 있어 금속 나노 와이어(nanowire)를 기반으로 하는 고기능성 나노 소재에 대한 연구들이 활발히 진행되고 있다. 그러나, 기존의 금속 나노 와이어의 경우 제조 공정의 복잡성, 유해 물질의 사용으로 인한 환경 오염의 유발, 정렬 및 제어의 어려움 등으로 인해 실질적인 응용에 있어 여러 단점들이 부각되고 있다. 이에 반해, 유기물을 활용한 하이브리드 나노 와이어의 경우 간단한 제작 공정, 친환경성, 유연성 등의 장점을 가지고 있어 차세대 기능성 소자로 각광받고 있다. 이에 본 연구에서는, 일반적으로 잘 알려진 생체 친화적 물질인 M13 박테리오파지를 이용하여 하이브리드 나노 와이어의 제작과 고에너지 분야에의 활용을 위한 여러 실험들을 수행하였다. 이를 위해, 음전하를 띄는 M13 박테리오파지와 금속 (Ag, Cu) 양이온 사이의 높은 전자 친화도와 무전해 도금 방법을 이용하여 20 nm 의 일정한 두께를 가지는 하이브리드 나노 와이어를 제작하였다. 제작된 나노 와이어는 TEM, SEM, XPS 등을 이용하여 물리 화학적, 구조적 특성들을 분석하였다. TEM 분석을 통해 나노 와이어의 제작에 사용된 금속의 격자구조를 관찰하였고, EDS-mapping 을 통해 M13 박테리오 파지의 표면에 금속이 고르게 분포되어 있음을 확인하였다. 또한 XPS 분석을 통해 제작된 나노 와이어의 품질에 대한 평가가 가능하였다. 또한, 산화된 하이브리드 나노 와이어가 가지는 높은 온도에서의 산소 전달 특징을 이용하여 고에너지 물질의 산화제로 활용하기 위한 점화 폭발 실험을 진행하였다. 점화 및 폭발 반응은 고속 카메라를 이용하여 촬영하였고, 시료의 길이에 따른 연소 시간의 측정을 통해 연소율을 계산하였다. 그 결과, 제작된 하이브리드 나노 와이어가 고온에서의 산소

제공을 통해 폭발력을 증대시키는 금속 산화제로 충분한 역할을 수행하고 있음을 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-95**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

1D Supramolecular Nanoplatform for Theranostics Based on Co-Assembly of Bioactive Amphiphiles

김인혜 이은지*

충남대학교 분석과학기술학과

A simple strategy for the preparation of multifunctional nanoparticles with potential diversification is presented using aqueous self-assembly of peptide amphiphiles (PAs) with precisely designed block. Versatile, one-dimensional (1D) supramolecular nanoplatform for personalized needs, particularly – theranostics, was fabricated by co-assembly of each functional PA, compensating for time-consuming and inaccessible chemical synthesis. Each PA was tagged with tumor cell-targeting peptide or was conjugated with ligand for paramagnetic metal ion (Gd^{3+}) for magnetic resonance (MR) imaging, respectively. The two PA types were co-assembled to integrate each PA function into the original 1D nanotemplates. Fibrils, driven by the assembly of PA with hydrophobic β-sheet–forming peptide block, were also utilized as a nanotemplate for drug loading within their robust core. The resulting 1D nano-aggregates allowed successful intracellular delivery of doxorubicin (DOX) to target cancer cells and contrast-enhanced MR imaging by high longitudinal (T_1) relaxivity of water protons. Correlation between the structural nature of fibrils formed by PA co-assembly and its diagnostic efficacy was elucidated. The co-assembly of PAs with desirable functions may thus be a useful strategy for the generation of tailor-made biocompatible nanomaterials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-96**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Injectable Hydrogel Based on Self-Assembling Short Pepetide Scaffolds

류주연 이은지[1,*]

충남대학교 분석과학기술대학과 [1]충남대학교 분석과학기술학과

Biomaterials made from self-assembling, short peptides and peptide derivatives have great potential to generate novel therapies in regenerative medicine. Peptide-based hydrogels have attracted extensive research interests due to the inherent properties of peptides, such as bioactivity, biocompatibility, and degradability. Among them, short peptide-based hydrogelators hold advantages because of the easy synthesis of short peptide and have been applied for drug delivery, cell culture, sensing and regenerative medicine. Meanwhile, many hydrogels have weak mechanical stability and high erosion rates, and therefore are unstable in vivo. This greatly hinders the application of hydrogel for drug delivery and controlled release. Therefore we aim to design short peptide-based self-assembled injectable hydrogel with moderate mechanical strength. In this study, diphenylalanine peptide (FF) derivatives are introduced that can increase mechanical strength of hydrogel through the additional non-covalent interactions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-97**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Bisphenol-A Novolac Polymer Developers for Thermal Printing Papers

권현진 최강훈 안병관*

가톨릭대학교 화학과

In order to replace a problematic BPA developer for thermal printing papers, Bisphenol-A novolac polymers were synthesized with bisphenol A and formaldehyde in the presence of acid catalyst. The effect of polymerization (reaction) time on the molecular weights, the thermal properties and the color-forming reaction properties was investigated. In addition, the preparation of thermal printing papers with these polymers was conducted and their developing capabilities including a static sensitivity were compared to those of BPA–based thermal printing papers.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-98**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Fabrication and Optical Properties of Hyperbranched Polymer Nanoparticles Containing Fluorescent Dyes

이예신 최강훈[1] 류영준[1] 안병관[1,*]

가톨릭대학교 자연과학부 화학과 [1]가톨릭대학교 화학과

Hyperbranched polymer nanoparticles containing fluorescent dyes were prepared by two different ways: (i) direct polymerization and (ii) surface modification. The chemical structure of the obtained polymer nanoparticles was confirmed by ^{1}H-NMR, FT-IR and elemental analysis. The size and shape of the nanoparticles were characterized by hydrodynamic size, zeta potential and FE-SEM analysis. The optical properties of colloidal nanoparticles were investigated by UV-visible absorption and photoluminescence spectroscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **POLY.P-99**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Visualization of Controlled Nano-Morphology in Nanowire-Based Active Layer via Electron Tomography

진선미 이은지[1,*]

충남대학교 분석과학기술대학원 [1]충남대학교 분석과학기술학과

The control of the active layer morphology is highly important to the photon to electron conversion in organic and hybrid solar cells with multi length scales. The direct visualization of three-dimensional bulk heterojunction morphologies has been challenging due to the complex molecular organization. In this presentation, we spatially resolve the morphology of hybrid thin-film based on the crystalline nanowires consisting of poly(3-hexylthiophene)-based polymers as the donor and quantum dots (QDs) as the acceptor via TEM tomography (TEMT). The hybrid nanowires are formed by conventional solvent mixing method, and then cast into thin-film for active layer. Interestingly, the crystallization of conjugated polymers are elucidated by the QDs nano-location within the hybrid nanowires in which the QDs are coaxial located along to the longitudinal and vertical nanowire axis. Therefore, the morphology of active layer and crystallinity of crystalline polymer could be demonstrated more easily by the QDs nano-location. The well-segregated p-n interface provide the continuous pathway for efficient charge energy transport. Therefore, 3D visualization and control of active layer morphology can reveal the intimate relations between hybrid active layer morphology and its device performance.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-1**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Chemical synthesis of cysteine and cysteine for pharmacy purposes

박수열* 김헌수

한국화학연구원 계면화학공정연구센터

L-cysteine has been widely used in medicines, cosmetics, and food additives. It has mainly been produced via acid or alkaline hydrolysis of human and animal hairs. However, these methods result in low yields and give rise to unpleasant odors and problems of waste treatment. In addition, products extracted from hair do not qualify for medical use because of sanitary problems. In our research, we, instead of hydrolysis of hairs, L-cystine was synthesized DL-2-amino-_2-thiazolin-4-carbonic acid (DL-ATC) to form L-cystine. The total cost for L-cystine synthesis using DL-ATC is favorable for the large-scale production in industry. L-Cysteine is one of two sulfur-containing amino acids which is used in diverse research fields including drug synthesis, food additives, and cosmetics additives.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **IND.P-2**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

아민기 치환을 통한 표면개질 유기흑색 안료의 분산성 및 내광성 평가연구

박수열[*] 김헌수 이병민

한국화학연구원 계면화학공정연구센터

표면개질된 유기흑색안료는 개질되지 않은 안료와 유사한 골격을 가짐에도 불구하고 표면개질된 블랙안료는 광학밀도, 낮은 유전상수 및 분산성 등의 물성이 우수하다고 보고되고 있다. 본 연구는 유기 블랙안료 표면에 다양한 유기아민을 부착시킴으로서 안료의 입자크기, 구조 및 형태를 변형시켜 분산보조제와 직간접적으로 호환성을 지니는 안료 잉크화에 관한 연구이다. 본 연구목적은 블랙매트릭스와 함께 사용할 수 있는 컬러필터용 흑색안료의 합성 및 물성평가를 통하여 분산성 및 내광성이 향상된 안료와 이들의 잉크조성물을 얻고자하는데 있다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-3**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

재활용 플라스틱을 이용한 인체 저유해성 스마트 자동차용 난연내장재 개발

박지영 조윤호 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

자동차 내장재로 사용되는 폴리에스터류로서 PET 부직포의 난연성 확보 및 시장 확대를 위해 인체 저유해성 난연제를 사용하여 스마트 자동차용 난연내장재를 개발하고자 한다. 이 난연내장재는 재활용 플라스틱을 이용(20~50% 사용)한 저가 난연칩으로 만들어진다. PET 는 연소성 물질이므로 난연성을 부여해야 한다. 이 방법 중 하나는 Br 계 난연제를 사용하는 것인데, Br 계 난연제는 인체 유해성 때문에 규제대상물질이므로 사용하여서는 안된다. 그래서 인체에 무해한 인계 난연제로의 대체가 요구된다. 본 연구에서는 폴리 에스터류 PET 와의 상용성이 확보되는 인계 난연제 종류를 선택하고 선정된 인계 난연제의 사용량 최소화의 배합비로 난연등급 1 등급(V-0 grade)을 확보하고자 한다. 이 난연 내장재는 자동차 내장재로서 난연 부직포 생산, 침구류(이불, 베개, 쿠션 등)의 난연 솜생산, 의료용 위생제품(아기 및 성인용 기저귀 등) 등에 활용할 수 있다.Acknowledgements : 연구는 2016 년도 계명대학교 산학협력선도대학(LINC) 육성사업 산학공동기술개발과제비 지원을 받아서 수행되었음.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-4**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mechanism Study on the Formation of N-Methyl-3-Pyrrolin-2-one from Purification of N-Methyl-2-Pyrrolidone

김송희 박유진 김진수[1,*]

한국화학연구원 고기능고분자연구센터 [1]한국화학연구원 화학소재연구단 정보전자폴리머연구센터

N-methyl-2-pyrrolidone (NMP) is a valuable solvent for eluent in industrial cleaners, photoresist strippers, photoresist coating solvent and size exclusion chromatography. Because NMP is synthesized by reaction of γ-Butyrolactone (GBL) and methylamine, these remain as impurities in synthesized NMP. NMP of exceptionally high purity for electronics applications could be obtained by several purification methods. Although hydrolysis of GBL with strong base, KOH has been successful to minimize GBL contents prior to the distillation of NMP, increasing basicity of the final distillate presumably due to CH_3NH_2 should be avoided. For solving this, *p*-toluenesulfonic acid (*p*-TSA) was chosen as an alternative catalyst for hydrolysis of GBL. In this case, decrease of GBL was not observed but increase of n-methyl-3-pyrrolin-2-one (NM3P) was monitored by Gas Chromatography (GC). Study was carried out to elucidate the mechanism of formation NM3P from NMP in the presence of *p*-TSA.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-5**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study on polymerization and properties of polyethylene wax by using metallocene catalysts

이상준 김성수 김인태*

광운대학교 화학과

In this study, we have studied properties of metallocene catalysts used for polymerization of polyethylene wax. We have evaluated hydrogen reactivity and studied on charactistics of polymerization effected by ligand structure of metallocene catalysts against Ziegler-Natta catalysts which are widely used for polymerization of polyethylene. We have also checked hydrogen used for chain transfer agent, molecular weight change and distribution by different ratios of ethylene gas. Finally, we suggest proper structure of metallocene catalysts for polymerization of polyethylene wax.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **IND.P-6**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Solubilities and anti-wear properties of thiadiazole and dithiocarbamate derivatives in base oil

이주연 김영준* 송재희[1]

충남대학교 화학과 [1]순천대학교 화학과

We synthesized some thiadiazole and dithiocarbamate derivatives containing long hydrocarbon chains.The solubilities of the compounds were compared in base oils such as DB-51, soybean, and 100N.Thiadiazole and dithiocarbamate derivatives were added to base oils to investigate the effect of its friction reducing properties using a 4-ball WSD tester.The solubilities of dithiocarbamate derivatives in the base oils were better than those of thiadiazole derivatives. The compounds containing oleoyl group rather than nonanoyl group gave good anti-wear properties. The solubilities and anti-wear properties were explained by the polarity of the compounds.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-7**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Adsorption of acetaldehyde using silica synthesized by sol-gel method

김문일 김수현[1] 류형석 김미리 임충선[2] 서봉국[3,*]

한국화학연구원 화학산업고도화센터 [1]부경대학교 공업화학과 [2]한국화학연구원 화학산업고도화 센터 [3]한국화학연구원 환경자원연구센터

Recently, the automobile industry is very large and tends to make the automobile and its materials more eco-friendly, sensitive, durable, light-weighted and economic. To fulfill one these new trends, development of adsorbents to reduce volatile organic compounds (VOC) and odorous gases is needed. Additionally, many countries have regulation of limits for VOC gas emission, and it is becoming stricter every year. One of the odorous VOC gas is acetaldehyde. Acetaldehyde can evaporate easily, and it not only has very stinging smell but also can harm the human body by inhaling it. Representative commercial adsorbents are activated carbons and silica gels. These samples feature large surface area, which is very connected to the good number of adsorption sites.In this study, silica xerogels were synthesized by sol-gel method to achieve higher surface area. And this sample was tested in a continuous bed system for adsorption of acetaldehyde, and was compared with the performances of commercial silica gel and activated carbon. Samples were analyzed by BET, in order to obtain the surface area. Concentration of inlet and outlet VOC gas from adsorption test tube were measured using TVOC detecting monitor.Silica synthesized by sol-gel method has higher surface area than commercial silica gel. Silica xerogel has better performance (Life time, amount of adsorption) on adsorption of acetaldehyde than those of commercial silica gel and activated carbon

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-8**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Surface treatment of the anatase type TiO2 powder with silica

양윤승 정헌주 김석찬* 박규순

국민대학교 화학과

Titanium dioxide(TiO2) is the most omportant white pigment used in the coatings industry. It is widely used because it efficiently scatters visible light, thereby imparting whiteness, brightness and opacity when incorporated into a coating. Titanium dioxide is commercially available in two crystal structures-anatase and rutile.Most commercial grades of titanium dioxide have inorganic and in some cases organic surface treatments. Inorganic surface modifiers most often are precipitated coatings of alumina and silica, which are meticulously controlles for type, amount, and method of deposition.In this study, the anatase type titanium dioxide surface-treated with SiO2 to be used for the white pigment.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-9**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Combined Computational and Experimental Study of Blue Iridium Complexes to develop an efficient, long-lasting blue PHOLED emitter

김소연 김진형 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

Organic light-emitting diodes are a major driving force of the current information display revolution due to their low power consumption and potentially long operational lifetime. Although electrophosphorescent organic emitters have significantly lower power consumption than fluorescent emitters, the short lifetime of electrophosphorescent blue devices has prevented their application in displays for more than a decade. Here, we demonstrate a novel blue electrophosphorescent device with a graded dopant concentration profile in a broadened emissive layer, leading to a lower exciton density compared with a conventional device. Thus, triplet-polaron annihilation that leads to long-term luminescent degradation is suppressed, resulting in a more than threefold lifetime improvement. A series of 4 novel blue phosphorescent dopants, namely, Ir(dmp)$_3$, Ir(dmp-Me)$_3$, Ir(dmp-CF$_3$)$_3$ and Ir(dmp-OMe)$_3$: dmp = 3-(2,6-dimethylphenyl)imidazo[1,2-f]phenanthridine, dmp-Me = 3-(2,6-dimethylphenyl)-7-methylimidazo[1,2-f]phenanthridine, dmp-CF$_3$ = 3-(2,6-dimethylphenyl)-7-(trifluoromethyl)imidazo[1,2-f]phenanthridine, and dmp-OMe = 3-(2,6-dimethylphenyl)-7-methoxyimidazo[1,2-f]phenanthridine have been designed and synthesized. Their thermal, photophysical and electrochemical properties were systematically investigated. Iridium complexes Ir(dmp)$_3$, Ir(dmp-Me)$_3$, Ir(dmp-CF$_3$)$_3$ and Ir(dmp-OMe)$_3$ emit bright sky-blue phosphorescence. Multi-layer phosphorescent organic light-emitting diodes using Ir complexes Ir(dmp)$_3$, Ir(dmp-Me)$_3$, Ir(dmp-CF$_3$)$_3$ and Ir(dmp-OMe)$_3$ as the triplet emitters and mCBP (3,3-di(9H-carbazol-9-yl)biphenyl) as the host have been fabricated. The device based on Ir(dmp-Me)$_3$ as an emitter shows a stable lifetime greater than 120 h at 2000 cd/m^2 (LT$_{70}$), which is one of the best results concerning the device lifetime.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-10**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Triphenylamine-Based Hole-Transporting/Exciton-Blocking Materials for High Thermal Stability and Power Efficient Phosphorescent OLEDs

김진형 조양진 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

A series of modified 4,4′-Cyclohexylidenebis[N,N-bis(4-methylphenyl)benzenamine] (TAPC), TAPC, SiTAPC, 2MeSi(TPA)$_2$, MeSi(TPA)$_3$ derivative have been tested as Hole-Transport Material for deep blue phosphorescent OLEDs. Systematic investigations of their thermal-, photophysical-, and Hole-transporting (HT) properties were successfully carried out. Low-temperature photoluminiscenec spectra indicate that all the prepared TAPC moieties maintained high triplet energy states up to 2.9 eV owing to the suppression of electron delocalization by silicon centre. Overally, all prepared compounds have relatively high triplet energy levels, which is compatible with the energy level of blue phosphorescent emitting layer in blue OLED device. TDDFT calculations were also performed to figure out their frontier orbital distributions and their transition states. In current-voltage (I-V) measurement (hole only devices (HOD)) to estimate their hole mobilities, the MeSi(TPA)$_3$ showed significantly higher current density than the other analogs. Finally the prepared compounds are applied as a hole transporting material to the emitting OLED device based on blue phosphorescent materials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-11**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Studies on the Photochemical Properties of the Iridium Carbene Complexes with Cyclometalated Methyl Imidazole Ligand for Stable Deep Blue Phosphorescent OLEDs

정원조 이종수 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

Achieving deep blue phosphorescence with high efficiency and brightness, together with long-term operational stability, remains a significant challenge. Improvement of the stability of blue phosphorescent dopant material is one of the key factor for real application of organic light-emitting diodes. In particular, imidazole ligand of Ir(III) complex tend to play an important role in the stability of blue phosphorescence. In addition, N-heterocyclic carbene (NHC) ligands, or $\mathrm{Ir(C{\wedge}C{:})_3}$ known for thermodynamically stable. Here, we focus on the stable blue phosphorescent emitters. We design and synthesis of some cyclometalated iridium complexes containing imidazole-type ligands: Iridium, *tris*[3,4-X(3-methyl-1*H*-imidazol-1-yl-2(3*H*)-*ylidene*)], (X=dibenzofurandiyl, phenylene, dibenzothiophenediyl, 9,9-dimethyl-9H-fluorene-3,2-diyl, 4-methylbenzothiadiazolediyl). We report a study of the photophysical properties of 5 cyclometalated Ir carbene complexes series.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-12**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Homoleptic Iridium(III) Complexes with Cyclometalated Carbene Ligand as Deep Blue Emitters for Phosphorescent Organic Light-Emitting Diodes

김진형 조양진 강상욱[1] 손호진[*]

고려대학교 신소재화학과 [1]고려대학교 소재화학과

The combination of both very high brightness and deep blue emission from phosphorescent organic light-emitting diodes (PHOLED) is required for display application, yet so far has not been reported. This difficulty comes from the absence of electron/exciton blocking layers (EBL) that are compatible with the high triplet energy of the deep blue dopant and the high frontier orbital energies of hosts needed to transport charge. Here, we show that N-heterocyclic carbene (NHC) Ir(III) complexes can serve as both deep blue emitters and efficient hole-conducting EBLs. We find that the two isomers of the dopant have high efficiencies that arise from the unusual properties of the NHC ligand. Our results represent an advance in blue-emitting PHOLED architectures and materials combinations that meet the requirements of many critical illumination applications

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **IND.P-13**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of Acryl Polyol for Window Decoration Film(WDF)

김도연[*] 박승현

애경화학기술원 연구소

Window Decoration Film(WDF) is a material for the cover glass, battery cover, camera lens glass print on a mobile display. WDF is capable of introducing a variety of colors and UV-pattern. It has good adhesion and differentiation, and direct printing, printing layers and bring a small interface has excellent transparency. In this study, We have developed Acryl resin for WDF by improving the adhesion and printability.

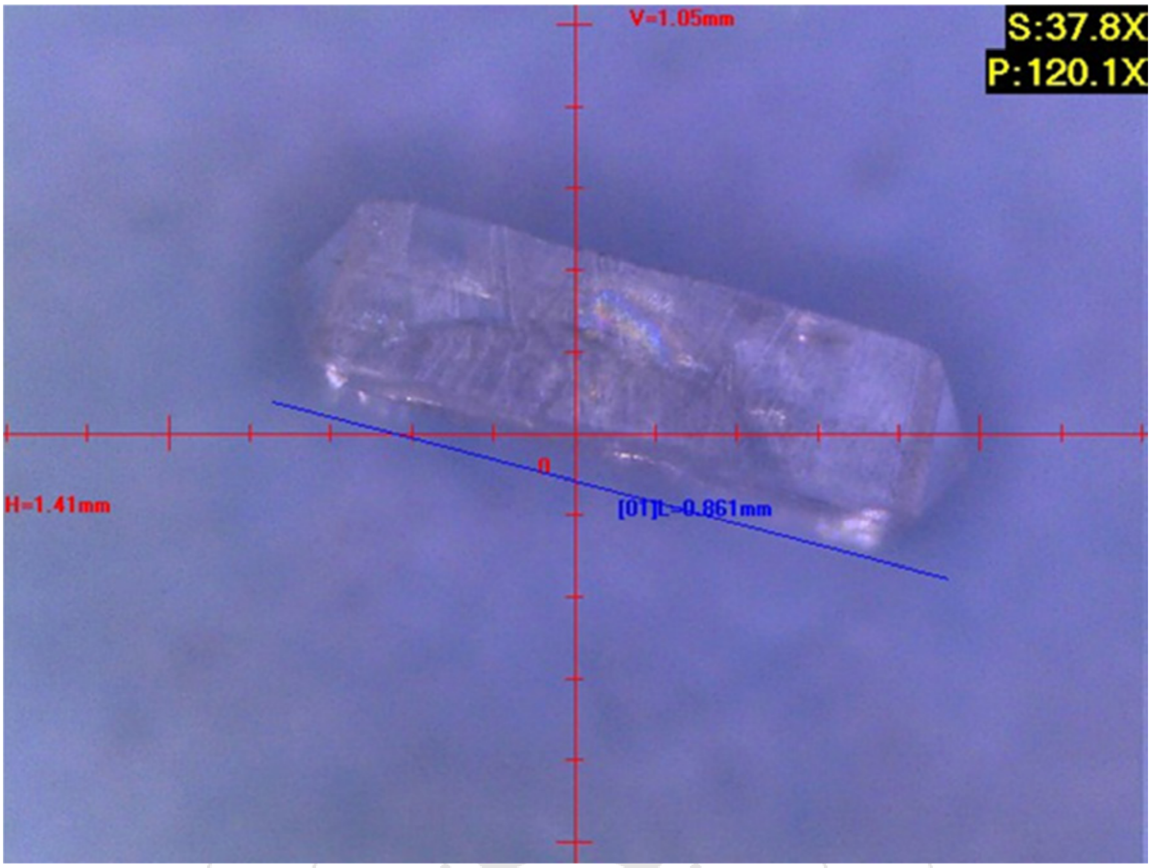
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **IND.P-14**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Single crystal structure of giant silicalite containing tetrapropylammonium hydroxide

조경철 조성준[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부

Single crystal structure of giant silicalite, 1.0 mm x 0.2 mm containing tetrapropylammonium hydroxide was determined readily with charge flipping method. The structure of occluded structure directing agent in the pore was obtained readily at the initial stage of refinement. The structure of silicalite was orthorhombic, $P2_12_12_1$ parameters of a= 19.9451 Å, b= 19.9611 Å and c= 13.3855 Å in which the chemical composition was $|C_{48}H_{112}N_4|$ $(SiO_2)_{96}$ with R_1/wR_2= 6.71/17.08 over 7513 reflections for $I > 3\sigma(I)$. The largest difference peak was 0.64 and the deepest hole was -0.69 e Å^3. The goodness-of-fitness index was 1.91. The final maximum (change/s.u.) was 0.0482.


V=1.05mm
S:37.8X
P:120.1X
H=1.41mm
0
[01]L=0.861mm

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-100**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Macrocyclic Nickel(II) Complex with 1,1’-Ferrocenedicarboxylate ligation

문성혁 김주창*

부경대학교 화학과

Macrocyclic nickel(II) complex, $\{[Ni(L)(fdc)]\cdot 3H_2O\}_n$ (1) (L = 1,4,8,11-tetraazacyclotetradecane, cyclam, fdc = 1,1’-ferrocenedicarboxylate ion) was prepared by the reaction of $[Ni(L)](ClO_4)_2$ and Na_2 fdc in DMF/H_2O. The complex 1 was characterized by EA, IR and TGA techniques. In addition, molecular structure was determined by single crystal X-ray diffraction methods. In 1, the fdc ligand bridges nickel(II) macrocycles to form an 1D coordination polymer in which 1D chains are connected each other by the mediation of lattice water molecules, resulting in the formation of 3D network. The torsional angle of two cyclopentadienyl (Cp) rings in 1 in the solid state was close to that of an anticlinal (eclipsed) structure. Details of the structural properties will be discussed in this presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-101**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

L-Aminoacid capped ZnS:Mn Nanocrystals as Effective Fluorescence Sensors and Photocatalysts in Aqueous Solution

박진우 황청수*

단국대학교 화학과

In this study, a water-dispersible ZnS:Mn nanocrystals (NCs) were synthesized by capping the surface with a simple L-aminoacid (alanine) at three different pH conditions to impart different surface properties to the NCs. The obtained ZnS:Mn NC products were optically and physically characterized by corresponding spectroscopic methods. The UV-Visible absorption spectra and PL emission spectra of the NCs showed broad peaks around 330 nm and 590 nm, respectively. The average particle sizes measured from the obtained HR-TEM images were about 5 nm, which were also well supported by the Debye-Scherrer calculations using the XRD data. Moreover, the surface charges and the degree of aggregations of the ZnS:Mn NCs were determined by electrophoretic and hydrodynamic light scattering methods respectively, indicating formation of agglomerates in water with negative surface charges. The negativley charged ZnS:Mn NCs showed an exclusive luminescence quenching for the copper (II) ion, and good photocatalytic activity on the phtodegration of methylene blue (MB) in aqueous solution.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-102**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mechanical Pressure-induced Luminescence Mechanochromism in CuI Coordination Polymer at Room Temperature

권은진 박현진 김진은* 장호재 임한수 김태호*

경상대학교 화학과

Copper(I) coordination polymer, $[Cu_2I_2\mathbf{L}_2]_n$ (CP **1**) was prepared by self-assembly reactions between CuI and 3-(2-(benzylthio)ethoxy)pyridine (**L**). CP **1** crystallizes in a monoclinic system, space group *C*2/*c* and has a one-dimensional loop-chain structure, where rhomboid Cu_2I_2 units are interconnected by **L**. CP **1** shows luminescence mechanocromism with color change from mint green to yellow upon pressure. PXRD and Raman studies reveal that changes of bond lengths in crystalline CP **1** in order to release internal energy by applied high pressure are the main cause of luminescence mechanochromism. The luminescence mechanochromic process of CP **1** maintains crystallinity with a small lattice distortion in spite of very high pressure and is a non-phase transition process. After the addition of several drops of acetonitrile to the ground and compressed samples, the original mint green emissive and crystalline state was restored. Therefore, the luminescence color conversion processes are fully reversible.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-103**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Reversible Crystal-to-Crystal Transformation and Solvato/Vapochromism of Cu (I) Coordination Polymers by Guest Exchange

박현진 권은진 장호재 임한수 김태호* 김진은*

경상대학교 화학과

Six Cu(I) Coordination Polymers (CPs) [CuI**L**]$_n$ (**1**), {[CuI**L**]·MeCN}$_n$ (**2**), [Cu_4I_4**L**$_2$]$_n$ (**3**), {[Cu_4I_4**L**$_2$]·$CHCl_3$}$_n$ (**4**), {[Cu_4I_4**L**$_2$]·CH_2Cl_2}$_n$ (**5**) and {[Cu_4I_4**L**$_2$]·C_6H_6}$_n$ (**6**) have been synthesized by self-assembly reaction of CuI and 4-(2-(cyclohexylthio)ethoxy)pyridine(**L**). CPs **1**-**6** are 1D loop chain structures. CPs **1-2** are based on Cu-I_2-Cu unit and CPs **3**-**6** are based on cubane-like Cu_4I_4 cluster nodes. Crystal-to-crystal transformations of CPs **1**-**6** were reversible under heat or appropriate solvent conditions (acetonitrile or chloroform or dichloromethane or benzene). Also, crystal transformations between CPs **1** and **3** occur through the addition of **L** or CuI. Moreover, CPs **4**-**6** exhibited reversible solvent exchange and crystal transformation by exposure to vapor of volatile organic compounds. In this presentation, the results of our investigation including synthesis, structural characterization, thermal and luminescent properties of six new Cu(I) coordination polymers are presented.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-104**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Crystal Structure and Luminescence Properties of Cu(I) Complexes Based on Sulfur Donor Ligands

임한수 권은진 박현진 장호재 김태호* 김진은*

경상대학교 화학과

The copper(I) iodide complexes containing a relatively simple sulfur atom such as *tert*-butyl(methyl)sulfane (**1**), cyclohexyl(methyl)sulfane (**2**) and benzyl(methyl)sulfane (**3**) have been synthesized and confirmed structurally characterized by single-crystal X-ray diffraction analysis. Complex **1** shows 1D ladder structure. Complexes **2** and **3** have cubane Cu_4I_4 cluster nodes. **2** shows a 1D chain structure while **3** shows a 0D discrete complex. Especially, **2** has a rare structure which shows that only Cu_4I_4 clusters are infinitively connected. Luminescence spectrum of the complex **1** exhibits an emission peak at 584 nm at room temperature. **2** and **3** show emission peaks at 498 nm and 530 nm, respectively.

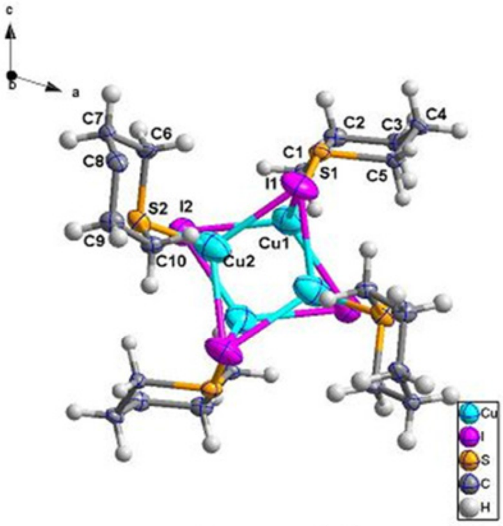
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-105**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Discrete Cubane Clusters, [$Cu_4I_4L^1_4$], [$Cu_4I_4L^2_4$] based on mono-dendate S atom ligands

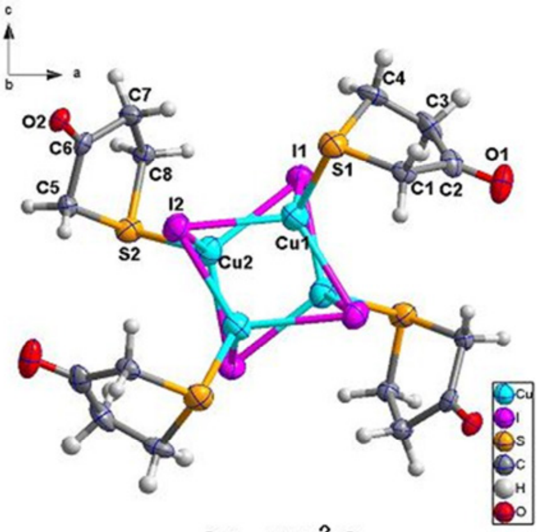
장호재 임한수 박현진 권은진 김태호* 김재상*

경상대학교 화학과

The reactions of CuI and each pentamethylene sulfide (**L**^{1}) and 3-tetrahydrothiophenone (**L**^{2}) by the ratio CuI : ligand = 1: 1 yield two discrete cubane clusters [$Cu_4I_4\mathbf{L}^1_4$] (**1**) and [$Cu_4I_4\mathbf{L}^2_4$] (**2**), respectively. Both solid powders were obtained without solvent under heat and ultra-sonication conditions. Both **1** and **2** show a discrete cubane Cu_4I_4 cluster structure having an inversion center as if they looked like four propeller wing shapes. **1** emits orange light while **2** emits yellow light under ultraviolet irradiation. **1** shows that a thermochromism phenomenon, i.e. hypsochromic (from orange to yellow) shift, occurs upon lowering temperature (from room temperature to 173K) whereas **2** does not show an emission color change. In this presentation, syntheses, structural characterizations, thermal and photoluminescence properties of two complex **1** and **2** are presented.



$[Cu_4I_4L^1_4]$



$[Cu_4I_4L^2_4]$

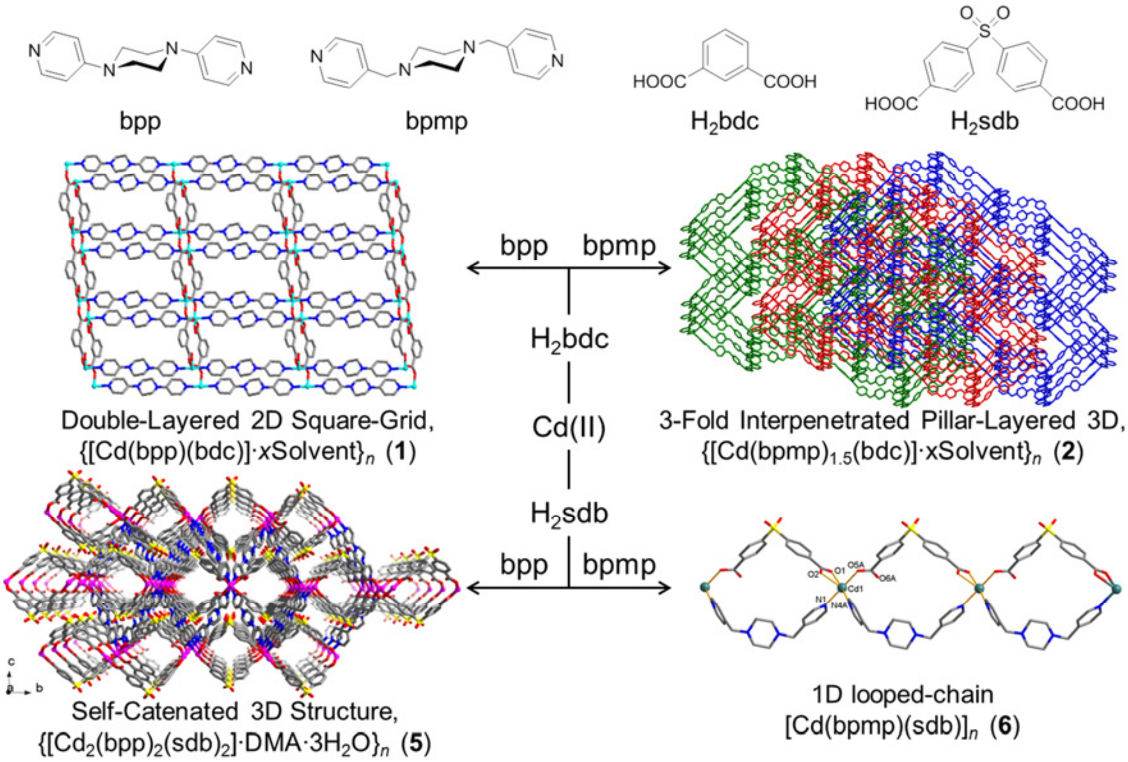
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-106**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Supramolecular Transition Metal Coordination Polymers Based on Dipyridyl Piperazine Ligands with Different Flexibility and Angular Dicarboxylic Acids

주희영 이심성*

경상대학교 화학과

The flexibility effect of dipyridyl piperazine ligands, bpp and bpmp, on the resulting metal-organic frameworks (MOFs) is reported. Binary ligand system of bipyridine derivatives (bpp and bpmp) and aromatic carboxylic acids (H_2bdc and H_2sdb) was employed to prepare MOFs (**1-6**). First, the reaction of bpp, $Cd(NO_3)_2{\cdot}6H_2O$, and H_2bdc yielded a double-layered 2D square-grid network $\{[Cd(bpp)(bdc)]{\cdot}x\text{Solvent}\}_n$ (**1**) in which the Cd(II) and bdc form a 1D double chain and further doubly linked by bpp in the axial positions. While, bpmp forms a 3-fold interpenetrated pillar-layered 3D framework $\{[Cd(bpmp)_{1.5}(bdc)]{\cdot}x\text{Solvent}\}_n$ (**2**). In, Cobalt(II) complexation, bpp and bpmp gave a double-layered 2D square-grid networks $\{[Co(bpp)(bdc)]{\cdot}x\text{Solvent}\}_n$ (**3**) and $\{[Co(bpmp)(bdc)]{\cdot}DMF{\cdot}0.5H_2O\}_n$ (**4**). In the reaction of bpp with $Cd(NO_3)_2{\cdot}6H_2O$ in the presence of H_2sdb, a self-catenated 3D structure $\{[Cd_2(bpp)_2(sdb)_2]{\cdot}DMA{\cdot}3H_2O\}_n$ (**5**) was isolated. When bpmp was used instead of bpp, $[Cd(bpmp)(sdb)]_n$ (**6**) adoption a 1D looped-chain structure was formed.


bpp
bpmp
H_2bdc
H_2sdb
HOOC
COOH
bpp
bpmp
H_2bdc
Cd(II)
H_2sdb
bpp
bpmp
Double-Layered 2D Square-Grid,
{[Cd(bpp)(bdc)]·xSolvent}$_n$ (**1**)
3-Fold Interpenetrated Pillar-Layered 3D,
{[Cd(bpmp)$_{1.5}$(bdc)]·xSolvent}$_n$ (**2**)
Self-Catenated 3D Structure,
{[Cd$_2$(bpp)$_2$(sdb)$_2$]·DMA·3H$_2$O}$_n$ (**5**)
1D looped-chain
[Cd(bpmp)(sdb)]$_n$ (**6**)
O2
O1
O5A
O6A
Cd1
N1
N4A
c
a
b

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-107**

발표분야: 무기화학

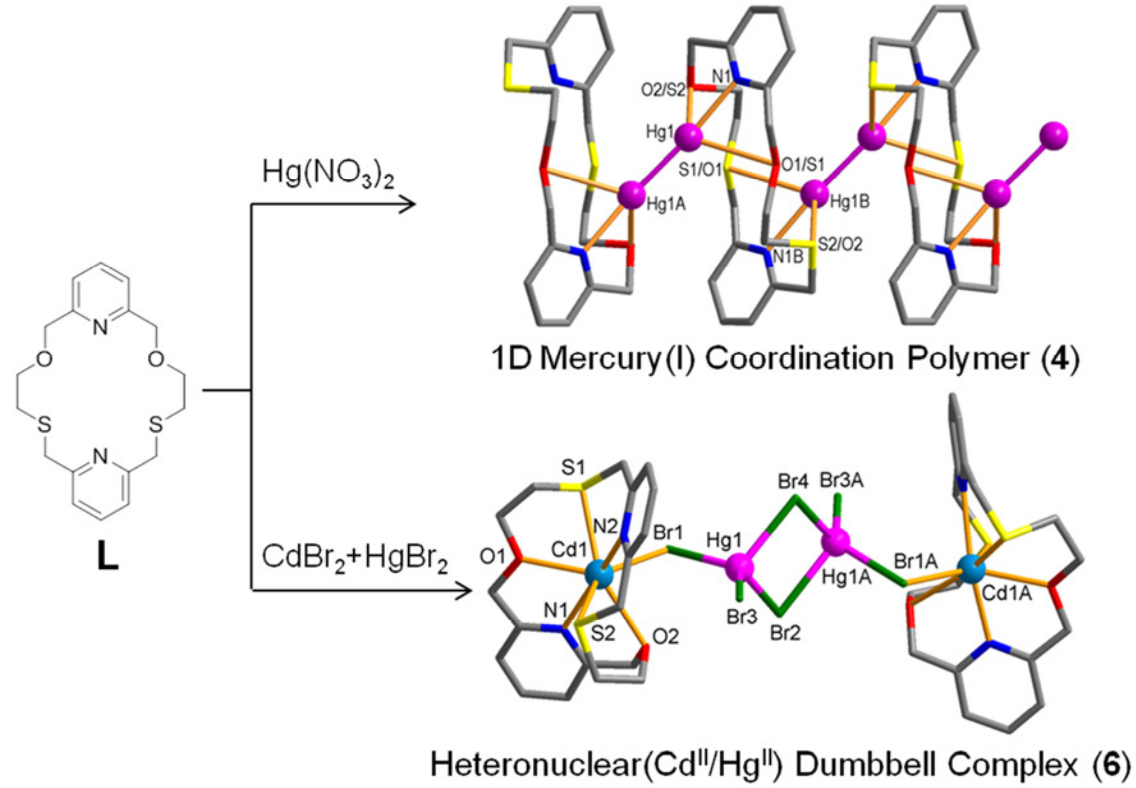
발표종류: 포스터, 발표일시: 목 11:00~12:30

Group 12 Metal Complexes of an 18-Membered $N_2O_2S_2$-Macrocycle: 1D Mercury(I) Coordination Polymer and Heteronuclear Dumbbell-Type Complex

서수진 이은지 이심성*

경상대학교 화학과

Group 12 metal (Zn^{2+}, Cd^{2+}, and Hg^{2+}) complexes of a newly designed $N_2O_2S_2$-macrocycle (**L**) including mercury(I) coordination polymer and dumbbell-type complex[1,2] were synthesized and structurally characterized. The reactions of $ZnBr_2$ and $CdBr_2$ with **L** afforded mononuclear complexes $[Zn(\mathbf{L})][ZnBr_4]$ (**1**) and $[Cd(\mathbf{L})Br_2]$ (**2**), respectively. When $HgBr_2$ was used, a dinuclear complex $[Hg^{II}{}_2(\mathbf{L})Br_4]$ (**3**) was obtained. While, $Hg^{II}(NO_3)_2$ gave a 1D coordination polymer $\{[Hg^{I}{}_2(\mathbf{L})](NO_3)_2\}_n$ (**4**) as a first example of the infinite macrocyclic mercury(I) complex, in which macrocycles are linked by the dimercury(I) ion (Hg^I-Hg^I). In addition, the reaction of a mixture of $ZnBr_2$ and $CdBr_2$ resulted in the isolation of two solubility-dependent Cd(II) complexes (**2** and **5**) with different stoichiometries including a half dumbbell-type complex $[Cd(\mathbf{L})(\mu\text{-}Br)(CdBr_3)]$ (**5**). While, one-pot reaction of **L** with a mixture of $CdBr_2$ and $HgBr_2$ afforded a dumbbell-type heterometallic bis(macrocycle) product $[(Cd\mathbf{L})_2(\mu\text{-}Hg_2Br_6)](Hg_2Br_6)$ (**6**), in which two terminal macrocyclic Cd(II) complexes are bridged by a dimercury(II) hexabromo cluster, Hg_2Br_6. The competitive binding abilities of mercury(II) and cadmium(II) to **L** in solution were also accomplished by the comparative NMR experiment and NMR titration. The results showed the relatively higher coordination affinity of Cd(II) toward the macrocycle than Hg(II), similar to that in the solid state.


L
Hg(NO3)2
CdBr2+HgBr2
O2/S2
N1
Hg1
S1/O1
O1/S1
Hg1A
Hg1B
N1B
S2/O2
1D Mercury(I) Coordination Polymer (4)
S1
N2
Br1
Br4
Br3A
Hg1
O1
Cd1
Hg1A
Br1A
N1
S2
O2
Br3
Br2
Cd1A
Heteronuclear(CdII/HgII) Dumbbell Complex (6)

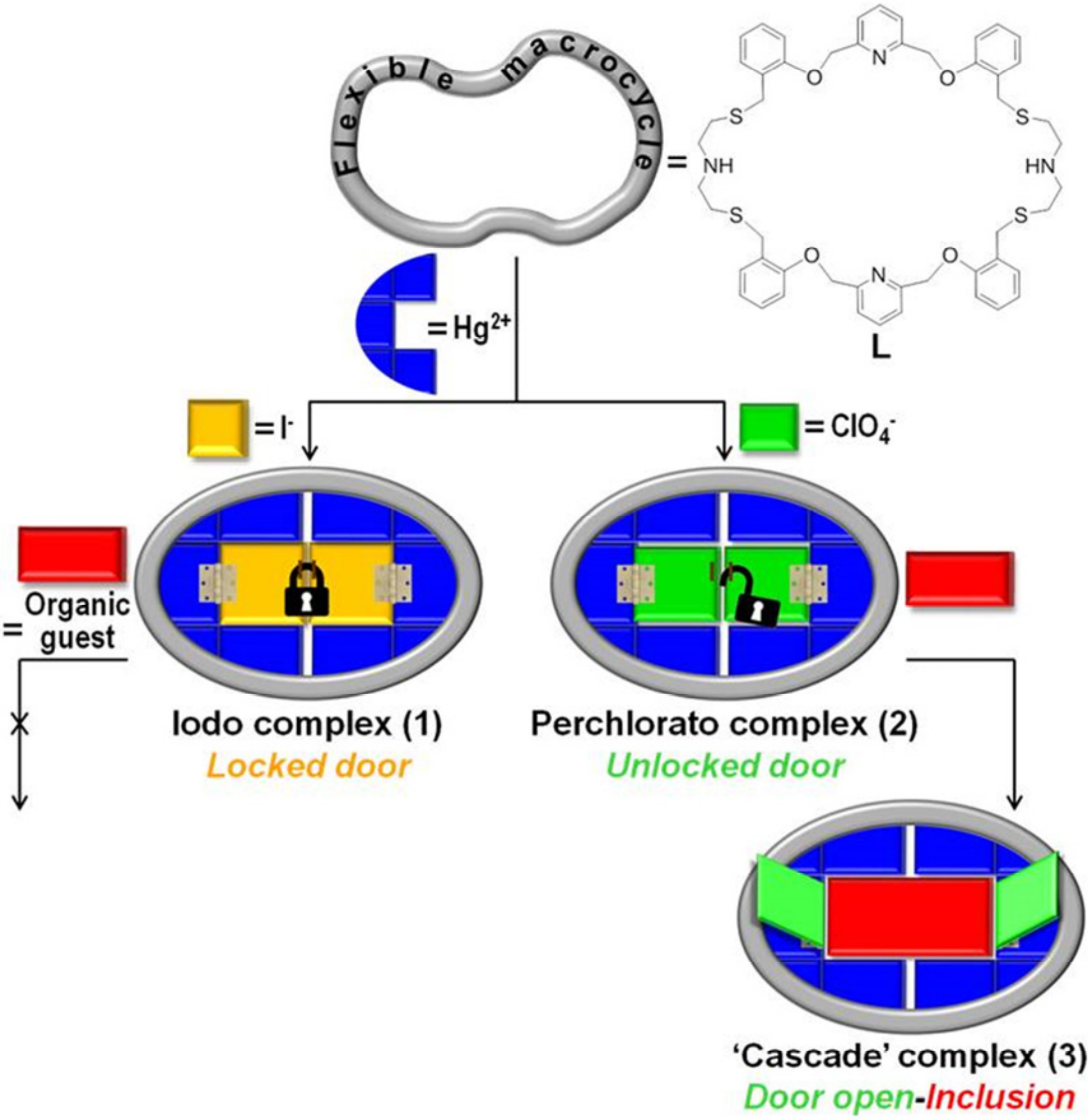
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-108**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Metallation-Mediated Induced Fit: Formation of Cascade Complex of Large Macrocycle Recognizing Organic Guest

이은지 **Yoichi Habata**[1] 이심성[2,*]

경상대학교 화학과 [1]Department of Chemistry, Toho University, Japan [2]경상대학교 화학과

In biological molecular recognition such as enzyme-substrate, some hosts change their shapes in order to bind selectively to a suitable guest via the induced fit. We have prepared a 40-membered $N_4O_4S_4$-macrocycle **L** though a 2:2 cyclization of the corresponding dithiol and dichloride as a minor product.[1] In extension, a macrocyclic host system exhibiting the metallation-mediated induced fit for the organic guest recognition is reported. The reaction of a large macrocycle **L** with HgI_2 afforded dinuclear complex $[Hg_2(\mathbf{L})I_4]\cdot 2DMSO$ (**1**), in which the Hg$\cdots$Hg distance in the macrocyclic cavity is 9.7 Å. Further reaction of **1** with 1,4-diazabicyclo[2,2,2]octane (dabco), a linker ligand, showed no reactivity with dabco such as locked door due to the inert nature of the coordinated iodo ligands. Meanwhile, reaction of **L** with $Hg(ClO_4)_2\cdot xH_2O$ afforded 1D coordination polymer with a rigidified dimercury(II) units $\{[Hg_2(\mathbf{L})(CH_3CN)(ClO_4)_3]ClO_4\cdot 2H_2O\}_n$ (**2**), in which the Hg$\cdots$Hg separation inside the cavity is 10.6 Å. Interestingly, reaction of **2** with dabco afforded a new type of dimercury(II) complex $[Hg_2(\mathbf{L})(\mu\text{-dabco})(ClO_4)_2](ClO_4)_2\cdot 2DMF\cdot 2ether$ (**3**), in which the space between two Hg atoms in the macrocyclic cavity is filled and linked with the dabco, adopting a Door open and inclusion of organic guest system.


Flexible macrocycle
=
NH
HN
S
O
N
L
= Hg2+
= I-
= ClO4-
= Organic guest
Iodo complex (1)
Locked door
Perchlorato complex (2)
Unlocked door
'Cascade' complex (3)
Door open-Inclusion

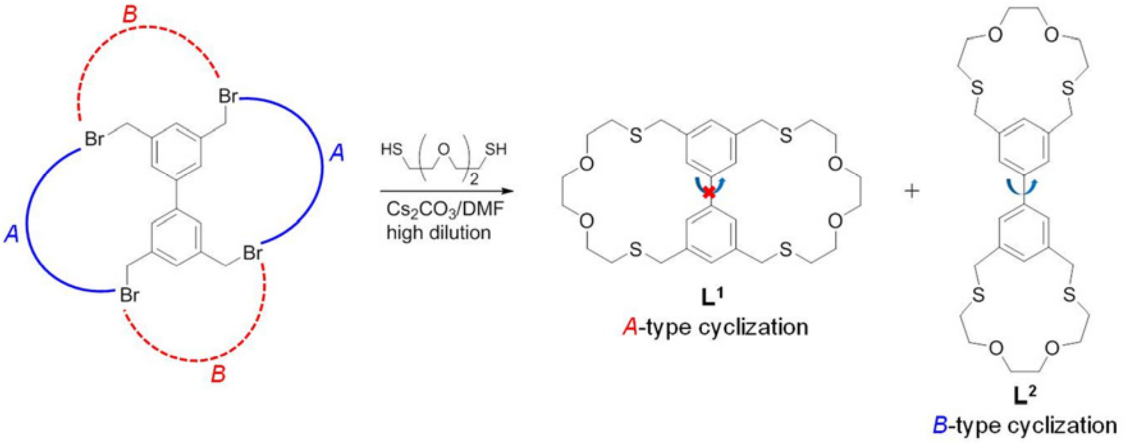
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-109**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Bis-Thiamacrocycle Isomers Incorporating Rotating Axis and Their Supramolecular Complexes

김슬기 이심성*

경상대학교 화학과

Coordination behaviors of the bis-thiamacrocycle isomers incorporating a biphenyl subunit exhibiting different rotating barriers are reported. For the synthesis of the bis-thiamacrocyclic ligands, the reaction of 3,3',5,5'-tetrakis(bromomethyl)biphenyl with two equiv of 3,6-dioxa-1,8-octanedithiol was carried out in the presence of Cs_2CO_3 in DMF under the high dilution condition. The ^{1}H NMR spectrum of this crude product shows the presence of two isomers $\mathbf{L}^1$ and $\mathbf{L}^2$ in via the A-type and B-type bicyclizations, respectively. However, the identification of each isomer by the NMR spectrum was not possible because of the very similar chemical shifts for the corresponding peaks. These two isomers in the mixture were separated using the column chromatography on silica gel. Fortunately, it was successful to obtain the single crystal structure of $\mathbf{L}^1$ which is a major product. Several soft metal complexes of $\mathbf{L}^1$ and $\mathbf{L}^2$ were isolated and their structural characteristics in solid state are discussed. For example, $\mathbf{L}^1$ reacts with copper(I) iodide to afford a 2D polymeric product $[(Cu_2I_2)\mathbf{L}^1]_n$ (**1**) in which the macrocycles are linked by square-type Cu_2I_2 clusters via the exocyclic coordination mode.


B
A
A
B
Br
Br
Br
Br
HS
O
2
SH
Cs2CO3/DMF
high dilution
S
O
O
S
S
O
O
S
L1
A-type cyclization
+
O
O
S
S
S
S
O
O
L2
B-type cyclization

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-110**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Polyrotaxane-Like 2D Coordination Polymers as Distortional Supramolecular Isomers

박인혁 주희영 Tun Seng Herng[1] 강윤지 이심성[*] Jun Ding[1] Jagadese J. Vittal[2]

경상대학교 화학과 [1]Department of Materials Science and Engineering, National University of Singapore, 119260, Singapore [2]Department of Chemistry, National University of Singapore, 117543, Singapore

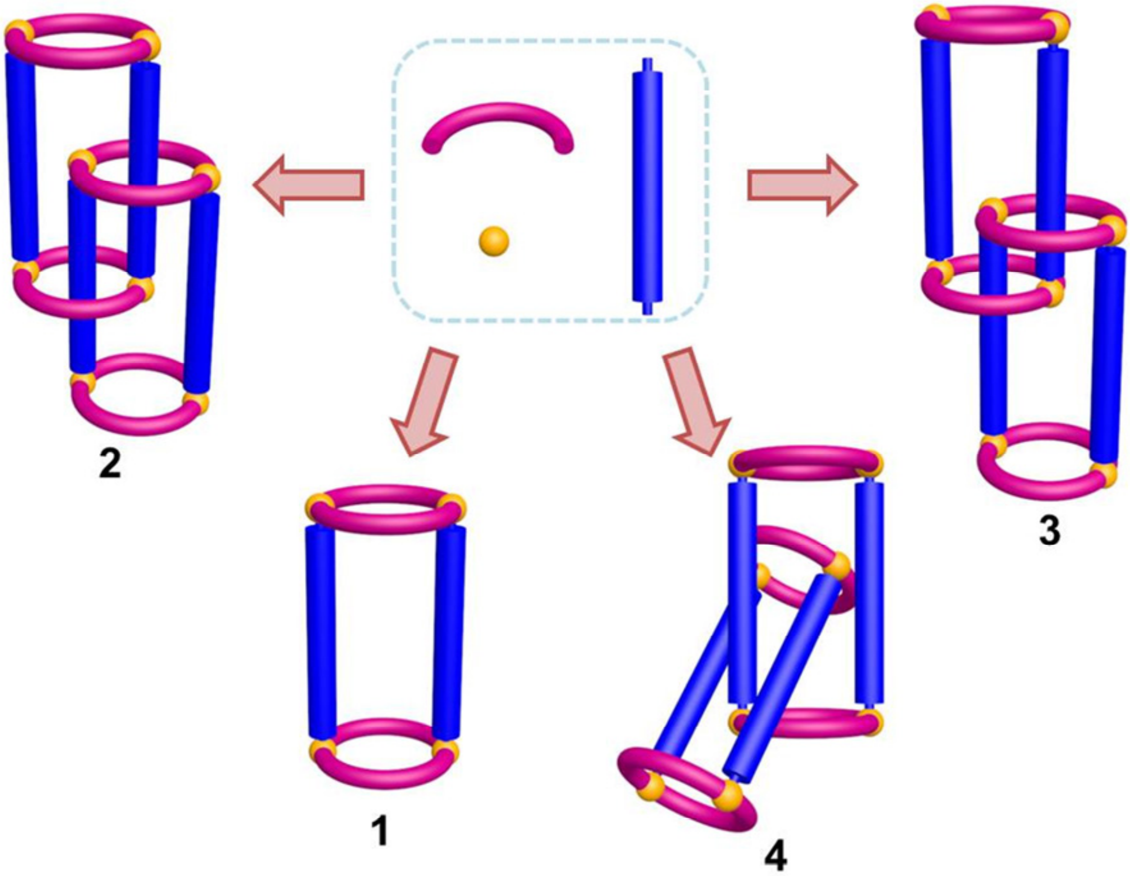
The term distortional isomerism is introduced to describe the structures of polyrotaxane 2D coordination polymers (CPs) that differ only by the relative positions in the neighboring entangled axles.[1] Such distortional supramolecular isomers may exhibit different physical properties and chemical reactivities.[2,3] Herein a bent dicarboxylate (sdb), a long dipyridyl spacer ligand (bpeb) with Co(II) has been used to design a two-dimensional (2D) sheets made up of rings and axles. Depending upon the experimental conditions used, seven CPs have been isolated which include a non-penetrated 2D sheet (**1**), two distortional supramolecular isomers (**2** and **3**), one two-fold diagonal/parallel interpenetrated 2D sheets (**4**), two more compounds isotypical to **2** but with two different guest solvents (**5** and **6**) and finally a polymorph **7** similar to **2**. They all have the same repeating units [$Co_2(bpeb)(sdb)_2$] based on paddlewheel structures. In all the structures, bpeb ligand has *trans,trans,trans*-conformation except **3** which has *trans,cis,trans*-conformation. The magnetic properties of **2** and **3** have been discussed.

References

[1] Park, I.-H.; Medishetty, R.; Lee, H.-H.; Mulijanto, C. E.; Quah, H. S.; Lee, S. S.; Vittal, J. J. *Angew. Chem., Int. Ed.* **2015**, *54*, 7313-7317.

[2] Park, I.-H.; Chanthapally, A.; Zhang, Z.; Lee, S. S.; Zaworotko, M. J.; Vittal, J. J. *Angew. Chem. Int. Ed.* **2014**, *53*, 414-419.

[3] Park, I.-H.; Mulijanto, C. E.; Lee, H.-H.; Kang, Y.; Lee, E.; Chanthapally, A.; Lee, S. S.; Vittal, J. J. *Cryst. Growth Des.* **2016**, *16*, 2504-2508.



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-111**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Snapshot and Crystallographic Characterization of Kinetic and Thermodynamic Products of Cadmium Iodide Complexes with NO_2S_2-Macrocycle

강윤지 박인혁* 이심성*

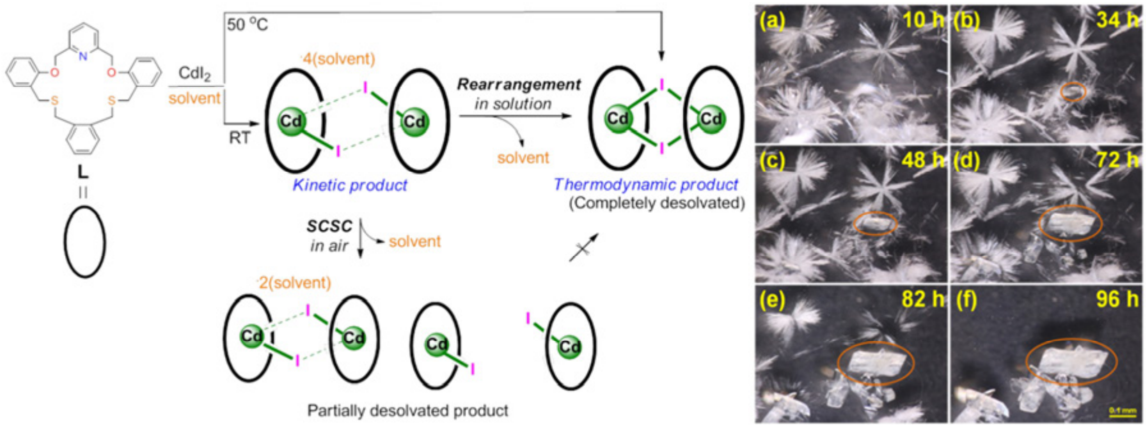
경상대학교 화학과

Similar to organic reactions, self-assembly of metallosupramolecule processes afford not only the thermodynamic product but also the kinetic product when the energy for the latter trapped in local minima.[1] Snapshot images, powder X-ray diffraction, and single crystal X-ray diffraction analysis as a function of time have shown that the self-assembly of a 19-membered NO_2S_2-macrocycle **L** with CdI_2 generates first a monomeric cadmium iodide complex and thereafter the dimeric analogue as kinetic and thermodynamic products, respectively (*see below*). In addition, removal of the lattice solvent molecules in the above kinetic complex in air motivates the displacement of the monomeric units showing partial structural changes in a single-crystal-to-single-crystal (SCSC) manner. The competitive NMR experiments for **L** between copper(I) and cadmium(II) were also carried out. The overall results agree with the solid state data that shows a higher affinity of copper(I) for **L** than does cadmium(II). Some other soft metals complexations of **L** both in solid and solution states are investigated and discussed.

References

[1] Martí-Rujas, J; Kawano, M. *Acc. Chem. Res*. **2013**, *46*, 493.

[2] Kang, Y.; Park, I.-H.; Ikeda, M.; Habata, Y.; Lee, S. S. *Dalton Trans*. **2016**, *45*, 4528.



L
CdI2
solvent
50 °C
RT
·4(solvent)
Cd
I
Kinetic product
Rearrangement
in solution
solvent
Thermodynamic product
(Completely desolvated)
SCSC
in air
solvent
·2(solvent)
Partially desolvated product
(a) 10 h
(b) 34 h
(c) 48 h
(d) 72 h
(e) 82 h
(f) 96 h
0.1 mm

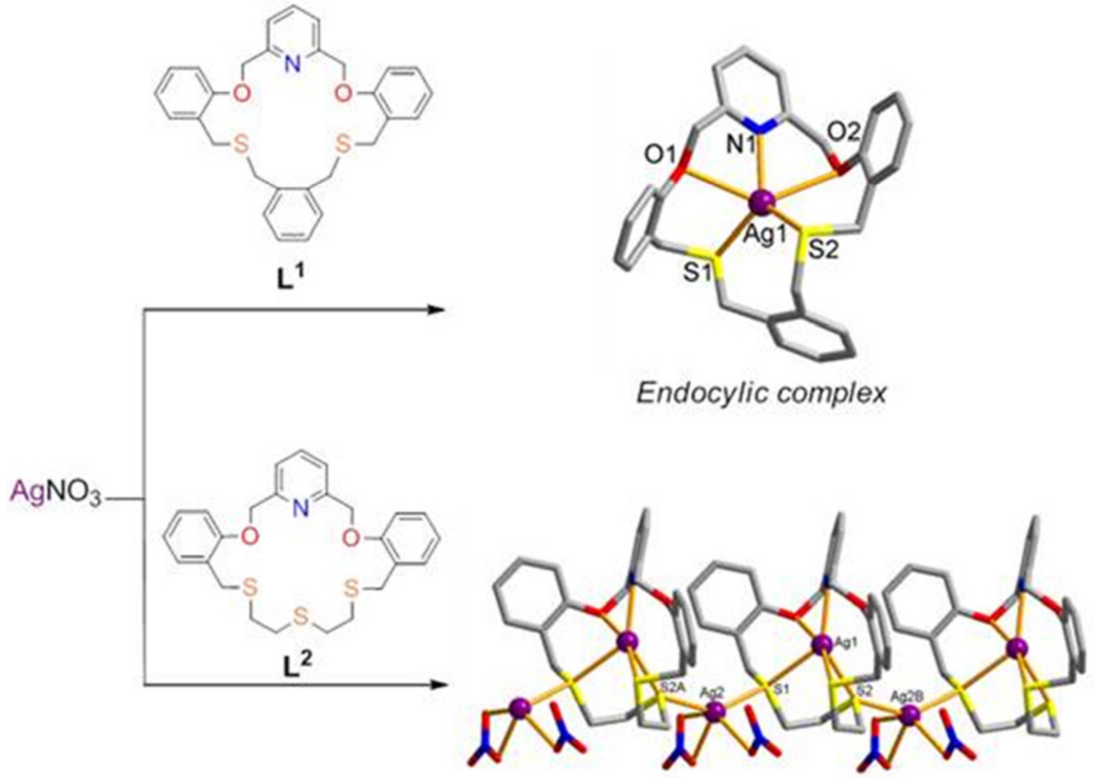
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-112**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ligand-Directed Endocyclic and Endo/Exocyclic Silver(I) Complexes of Thiaoxaaza-Macrocycles: Crystallographic and NMR Studies

박인혁 강윤지 주희영 이은지 김슬기 이심성*

경상대학교 화학과

A comparative investigation of the coordination behaviour of a 19-membered NO_2S_2-macrocycle (**L**^{1}) and a 20-membered NO_2S_3-macrocycle (**L**^{2}) is reported. On silver(I) complexation, **L**^{1} yields a discrete endocyclic mononuclear complex, while **L**^{2} affords a one-dimensional coordination polymer in which the endo-coordinated macrocyclic complex units are linked by silver(I) ions outside the cavity via the endo/exo-coordination. The larger ring cavity with a flexible nature of **L**^{2} may induce the weaker endocyclic complexation and attribute to the exocyclic coordination as well. In the NMR titration studies for the corresponding complex system, however, no evidence of the exocyclic coordination was observed. Instead **L**^{1} and **L**^{2} form a stable endocyclic 1:1 silver(I) nitrate complex, with the higher affinity of the former one.



Endocylic complex

Endo/exocyclic 1D coordination polymer

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-113**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Influence of the Degree of Interpenetration on the [2+2] Photo-Cycloaddition Reaction inside MOFs

박인혁 Caroline Evania Mulijanto[1] 강윤지 이은지 Anjana Chanthapally[1] 이심성[*] Jagadese J. Vittal[1]

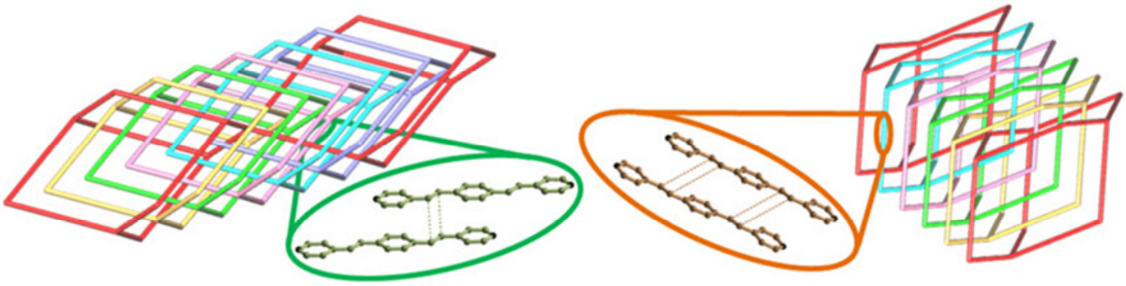
경상대학교 화학과 [1]Department of Chemistry, National University of Singapore, Singapore

The degree of interpenetration is known to influence the gas sorption, catalytic, magnetic and non-linear optical properties, chirality, sensing of various molecules but not solid-state [2+2] photo-cycloaddition reaction. In our previous solvothermal reaction in dimethylacetamide (DMA) as one of the solvents, a photoreactive six-fold interpenetrated MOF with **dia** topology, [Zn(bpeb)(bdc)] (**1**) [bpeb = 1,4-bis[2-(4'-pyridyl)ethenyl]benzene; bdc = 1,4-benzenedicarboxylicacid] was isolated. Due to slip-stacked alignment of a dipyridyl ligand with two conjugated olefin bonds, [2+2] cycloaddition reaction occurs under UV light leading to the formation of organic polymer ligand fused with coordination polymer, **2**.[1] On the contrary, under the similar conditions when diethylformamide (DEF) was used instead of DMA, a five-fold interpenetrated structure, **3** with the same **dia** topology was obtained.[2] This has been found to be photostable as also predicted from the analysis of solid state structure. All the solids show interesting photoluminescence properties and the emissions were preferentially quenched by curcumin to make these materials as potentially useful sensing agents.

References

[1] Park, I.-H.; Chanthapally, A.; Zhang, Z.; Lee, S. S.; Zaworotko, M. J.; Vittal, J. J. *Angew. Chem. Int. Ed.* **2014**, *53*, 414-419.

[2] Park, I.-H.; Mulijanto, C. E.; Lee, H.-H.; Kang, Y.; Lee, E.; Chanthapally, A.; Lee, S. S.; Vittal, J. J. *Cryst. Growth Des.* **2016**, *16*, 2504-2508.



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-114**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation of tetrazole-thiolato Pd(II) complexes using organic tetrazole-thiones

김용주* <u>김남수</u> 이순원[1]

강릉원주대학교 화학과 [1]성균관대학교 화학과

Reactions of dialkyl Pd(II) complexes with organic tetrazole-thiones {S=[C{HN4(R)}] afforded new tetrazole-thiolato Pd(II) complexes. The isolated complexes were determined by IR and NMR spectroscopy and X-crystallographic analyses. As the starting material, new diethyl Pd(II) complex with allyldiphenyl phosphines was prepared from the reactions of Pd(acac)2 and allyldiphenyl phosphine in the presence of AlEt2(OEt). Experimental detail will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-115**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gas Sorption Properties of Zn-MOFs with Lewis Basic N-rich Channels

김현철 김성진[1] 김영미[2] 허성*

한국외국어대학교 화학과 [1]이화여자대학교 화학과 [2]이화여자대학교 화학-나노과학과

Lewis basic heteroatoms located inside the channels of metal-organic frameworks (MOFs) are active sites for catalysis and gas sorption. We prepared four new Zn-MOFs containing C_{2h}-symmetric dicarboxylate bridging ligands, 3,3'-(pyrazine-2,5-diyl)dibenzoate (3,3'-PDBA) or terphenyl-3,3'-dicarboxylate (3,3'-TPDC), and two different pyridine-based pillars, 1,2-bis(4-pyridyl)ethane (bpa) or 1,2-bis(4-pyridyl)ethylene (bpe). The resulting four isostructural Zn-MOFs of the general formula of $[Zn_2(\text{dicarboxylate})_2(\text{bpa})]$ or $[Zn_2(\text{dicarboxylate})_2(\text{bpe})]$ displayed diamond-like framework geometry. Both $[Zn_2(\text{3,3'-PDBA})_2(\text{bpa})]$ and $[Zn_2(\text{3,3'-PDBA})_2(\text{bpe})]$ contain Lewis basic N atoms inside channels compared with $[Zn_2(\text{3,3'-TPDC})_2(\text{bpa})]$ and $[Zn_2(\text{3,3'-TPDC})_2(\text{bpe})]$. $[Zn_2(\text{3,3'-PDBA})_2(\text{bpa})]$ showed selective sorption of CO_2 over H_2, N_2 and CH_4. Furthermore, the adsorption and desorption isotherms for CO_2 showed a significant hysteretic behavior possibly due to breathing effect of the activated form. Therefore, the former two Zn-MOFs are better adsorbents for quadrupolar CO_2 gas. Further differences in gas sorption abilities because of the different flexibility between bpa and bpe pillars will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-116**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of 4,4-Disubstituted-2,6-bis(trimethylsilyl)dithienosilole

박지영 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

3,3’-Dibromo-5,5’-bis(trimethylsilyl)-2,2’-bithiophene was synthesized by the substitution reaction of 3,3’,5,5’-tetrabromo-2,2’-bithiophene using *n*-butyllithium and chlorotrimethylsilane. 4,4-Disubstituted-2,6-bis(trimethylsilyl)dithienosilole was synthesized by the intramolecular cyclization reaction of 3,3’-dibromo-5,5’-bis(trimethylsilyl)-2,2’-bithiophene using *n*-butyllithium and dichlorodisubstitutedsilane. 2,6-Dibromo-4,4-disubstituteddithienosilole was synthesized by the substitution with NBS to 4,4-disubstituted-2,6-bis(trimethylsilyl)dithienosilole. The obtained dithienosilole derivatives are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by ^1H, ^{13}C NMR, and FT-IR spectroscopies along with TGA. We also studied the electronic properties by UV-vis absorption, excitation, fluorescence emission spectroscopic methods, and cyclic voltammetry, in particular.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-117**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Photophysical Properties of Deep Blue Phosphorescent Iridium(III) Complexes with *o*-Carborane

김민지 이형동 박재영 **KUMAR AJAY** 이민형*

울산대학교 화학과

Iridium(III) complexes with *o*-carborane (1,2-*closo*-$C_2B_{10}H_{12}$) has recently emerged as a new class of phosphorescent emitters in OLEDs due to steric bulkiness and electronic effect of an *o*-carborane cage. In particular, the introduction of *o*-carborane enabled facile tuning of emission color of Ir(III) complexes by inductive electron-withdrawing and conjugation effect of *o*-carborane. Because of high demand in optoelectronic applications, the development of novel deep blue phosphorescent emitters is being actively investigated. In this study, we newly designed two iridium(III) cyclometalates in which an *o*-carborane unit is introduced in the dfppy (2-(4,6-difluorophenyl)pyridinato-C^2,N) ligand. The resulting complexes showed blue-shifts in phosphorescence compared to that of the corresponding parent FIrpic and FIr6 complex, respectively. Details of synthesis, characterization, and photophysical properties of deep blue emitters will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-118**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Turn-On Phosphorescent Sensing of Fluorides by Ir(III) Cyclometalates with *o*-Carborane

NGUYEN VAN NGHIA 이형동 박재영 **KUMAR AJAY** 이민형*

울산대학교 화학과

Fluoride sensing has received great attention during the last decade because of the detrimental effect of fluoride in physiological systems. In particular, detection of fluoride at low concentrations, such as the parts per million level, in aqueous media has been an important issue from a practical point of view. In this regard, phosphorescent sensors based on heavy-metal complexes conjugated with a receptor unit have recently been of great interest due to their advantageous photophysical properties. As a novel class of "OFF-ON"-type phosphorescent sensors, heteroleptic tris-cyclometalated Ir(III) complexes with *o*-carborane (*closo*-1 and 2) were prepared in this study. These complexes were shown to be almost nonemissive in an aqueous medium, but became highly emissive upon deboronation of the *closo*-carborane cage by fluoride. This allowed selective, turn-on phosphorescent sensing of fluoride in aqueous medium at the ppb level. Details of synthesis, characterization, and photophysical properties of deep blue emitters will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-119**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoinduced Reduction of Cu^{2+} paddlewheels in Coumarin-tethered Metal-Organic Polyhedra

배재연 박진희[1,*]

DGIST 신물질과학전공 [1]DGIST 신물질과학과

Since the last two decades, the various structural metal-organic polyhedra (MOPs) have been intensively studied owing to their potential applications such as gas storage, catalysis, drug delivery, etc. However, post-synthetic modification of MOPs has mainly focused on adding additional functional groups on their organic linkers. This presentation will include a new strategy for reversible control of the oxidation states of Cu^{2+} in MOPs. The optically responsive MOPs were prepared by using optically responsive coumarin derivatives as organic linkers (coumarin-MOPs). Because coumarin can be excited by UV irradiation, the transferred amount of electrons from photosensitizers to Cu^{2+} paddlewheels was effectively controlled. Sequential reduction of Cu^{2+} was failed in MOPs that do not contain any optically responsive moieties. Photo-induced catalytic activity of coumarin-MOPs is under examination.

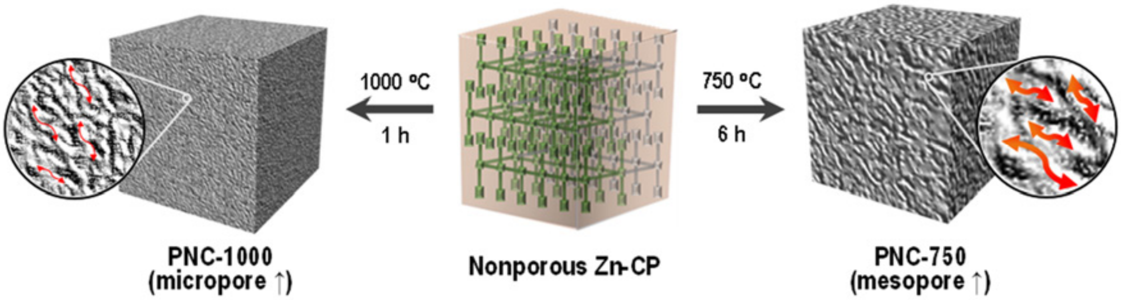
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-120**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Upcycling of nonporous coordination polymers: controllable-conversion toward porosity-tuned N-doped carbons and their electrocatalytic activity in seawater batteries

정성은 문회리[1,*]

UNIST 친환경에너지공학부 [1]UNIST 화학과

Herein, we report the preparation of highly porous N-doped carbons (PNCs) via thermolysis of nonporous Zn-based coordination polymers (CPs) constructed with nitrogen-containing ligands. So far, the thermal conversion of Zn-CPs, including metal–organic frameworks (MOFs), has mainly yielded microporous carbon materials, and to change the textural properties of end carbons, new CPs/MOFs with different properties were introduced. However, present studies show that just varying the conversion conditions of a parent CP results in porosity-tuned PNCs, in which especially mesoporosity is developed, and this is applicable for even nonporous CPs. This is conducted based on the understanding of conversion phenomena which is that during thermal conversion of Zn-based CPs, the in situ generated Zn metal species act as porogens and their agglomeration can be controlled by the reaction conditions. Different reaction temperatures, ramping rates and retention times allow control over the ratio of micro- to meso-pore volume, while a slower ramping rate and longer retention time at lower heating temperature induced the agglomeration of the porogens, yielding greater mesoporosity, and holding the Zn-CPs at high temperature for a short period afforded the micropore-dominant PNCs due to rapid porogen elimination. The superiority of the mesopore-developed PNCs as electrocatalysts, attributed to greater mass-transport-accessible surfaces, was examined for the electrodes in a rechargeable seawater battery system as an example of a practical application. Therefore, our synthetic approach provides a facile method for the preparation of PNCs with suitable hierarchical pore distributions for use as energyrelated materials without exerting significant effort in the design of coordination compounds.


1000 ºC
1 h
750 ºC
6 h
PNC-1000
(micropore ↑)
Nonporous Zn-CP
PNC-750
(mesopore ↑)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-121**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Peroxidase activity of transition metal complexes in group 8 through kinetic study

김오연 이홍인*

경북대학교 화학과

Peroxidase (peroxide oxidase) is a family of the enzymes that catalyze oxidation reactions using hydrogen peroxide. Peroxidase activity is widely applied for many important usages such as industrial waste waters, chemical sensors, immunohistochemistry, and ELISA studies. It has been found that many transition metal complexes such as iron complexes have shown the peroxidase activities. However, the peroxidase activity by ruthenium complexes are very rare. We have tested the peroxidase activity of ruthenium complexes by using guaiacol, ABTS (2,2’-azino-bis(3-ethyl-benzothiazoline-6-sulphonic acid), and methyl orange as substrates, and found the peroxidase activity of ruthenium complexes. In this study, we compare the activities of iron and ruthenium complexes containing H2EBPP (=N,N'-(ethylene-di-p-phenylene)bis(pyridine-2-carboxyamide)) ligand.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-122**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cobalt(II) complexes containing bispyrazolyl ligand: Synthesis, structure and methyl methacrylate polymerization

신수진 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

We have synthesized several new Co(II) complexes with ligands L_n ($L_n = L_A – L_D$) where L_A = (N,N-bis((1H-pyrazol-1-yl)methyl)-3,5-dimethylbenzenamine), L_B = (N,N-bis((3,5-dimethyl-1H-pyrazol-1-yl)-3,5-dimethylbenzenamine), L_C = (N,N-bis((1H-pyrazol-1-yl)methyl)-4-methoxybenzenamine), L_D = (N,N-bis((3,5-dimethyl-1H-pyrazol-1-yl)- 4-methoxybenzenamine). All ligands and Co(II) complexes were characterized by ^{1}H-NMR, ^{13}C-NMR, IR, and Elemental Analyzer. Molecular structures of complexes were determined by X-ray single crystal diffraction. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were also investigated at 60 ^{o}C.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-123**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Structural Characterization of Cobalt(II), Zinc(II), Copper(II), and Cadmium(II) Complexes Containing 4-Bromo-*N*-(2-pyridinylmethylene)benzenamine

박수현 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

The reaction of [$CoCl_2.6H_2O$], [$ZnCl_2.xH_2O$], [$CuCl_2.2H_2O$] and [$CdBr_2.4H_2O$] with ancillary ligand, 4-bromo-*N*-(2-pyridinylmethylene)benzenamine (L_A) in ethanol, respectively gave the corresponding complexes, i.e. [L_ACoCl_2], [L_AZnCl_2], dimeric [$L_ACu(\mu\text{-}Cl)Cl]_2$ and [L_ACdBr_2], respectively. Molecular structures of [$L_ACu(\mu\text{-}Cl)Cl]_2$ was characterized by X-ray crystallography. The catalytic activity of complex toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were also monitored at 60 ^oC.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-124**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, structure and reactivity of cadmium(II) complexes with N, N',N"-tridentate ligands

허정 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

We have synthesized and characterized a series of new cadmium(II) complexes, namely [L_nCdBr$_2$] with ligands L_n (L_n = L_A – L_D), where [L_A = (E)-2-(piperidin-1-yl)-N-(pyridin-2-ylmethylene)ethanamine), L_B = (E)-2-morpholino-N-(pyridin-2-ylmethylene)ethanamine), (L_C = (E)-2-methoxy-N-(pyridin-2-ylmethylene)aniline), (L_D = (E)-2-(methylthio)-N-(pyridin-2-ylmethylene)aniline). New Cd(II) complexes are characterized by spectroscopic methods such as 1H NMR, 13C NMR, IR, and elemental analysis. Molecular structure of [L_ACdBr$_2$] and [L_BCdBr$_2$] were determined by X-ray single crystal diffraction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-125**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of cobalt(II) complexes containing N,N, N', N"-tetradentate bispyrazolyl ligand

서재영 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New complexes [LnCoX] (Ln = L_A, L_B, L_C, L_D; X = Cl, NO_3) were synthesized by the reaction of starting metal material [$CoCl_2.6H_2O$] or [$Co(NO_3)_2.6H_2O$] with the corresponding N,N-bis((1H-pyrazol-1-yl)methyl)-2-(piperidin-1-yl)ethan-1-amine (L_A) and N,N-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-2-(piperidin-1-yl)ethan-1-amine (L_B) and N,N-bis((1H-pyrazol-1-yl)methyl)-2-(pyrrolidin-1-yl)ethan-1-amine (L_C) and N,N-bis((1H-pyrazol-1-yl)methyl)-1-(pyridin-2-yl)methanamine (L_D), respectively followed by addition of $Na(BPh)_4$. Molecular structures of these complexes were characterized by X-ray diffraction.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-126**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gas sorption properties of S/N-doped microporous carbons derived from $In(tdc)_2$-MOF

최인환 허성*

한국외국어대학교 화학과

Indium sulfides nanoparticle-embedded S/N-doped microporous carbons were simply prepared through a carbonization of In(III)-based metal-organic framework (In-MOF), $[Et_2NH_2][In(tdc)_2]\cdot DEF$, which contains 2,5-thiophenedicarboxylate (tdc^{2-}) bridging linker as a source of S-dopant. The anionic framework of $In(tdc)_2$ is charge balanced by $Et_2NH_2^+$ counter-cation a potential N-dopant. Simultaneous embedding of In-based nanoparticles, S-doping and N-doping were achieved in a single step carbonization of In-MOF. Three porous carbon materials PCM-700, PCM-800, and PCM-900 were obtained from carbonization at 700 °C, 800 °C, and 900 °C, respectively. These carbon materials were fully characterized by PXRD, SEM, TEM, XPS, and Raman spectroscopy. The gas sorption analysis was also performed using N_2, CO_2, and H_2 at suitable temperatures. They are good CO_2 sorbents due to the presence of Lewis basic S-dopants.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-127**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of copper(II) complex bearing (1*R*,2*R*)-N'- (2,4,6-trimethoxybenzyl)-N"-benzylcyclohexane-1,2-diamine and its application toward asymmetric henry reaction

천민경 정종화*

경북대학교 화학과

Novel Cu(II) complex bearing (1*R*,2*R*)-N'-(2,4,6-trimethoxybenzyl)-N"- benzylcyclohexane-1,2-diamine was synthesized and applied to enantioselective Henry reaction. New copper complex was characterized by X-ray diffraction. In the x-ray structure, four diastereomeric molecules were cocrystalized. They are divided into two on the basis of the nitrogen configuration. One type of complexes has two nitrogens that one nitrogen is R configuration and another is S configuration ($S_{N'}R_{N''}$-1R,2R) while the other type has SR configuration nitrogens ($S_{N'}R_{N''}$-1R,2R). In $S_{N'}R_{N''}$-1R,2R diastereomers, there is difference in the three-demensional structure. While one complex has exo position at 4-methoxy group, another has endo position. SNRN-1R,2R diastereomers were same. The synthesized dichlorocomplexes and their diacetato derivates were investigated for asymmetric nitroaldol reaction between benzaldehyde and nitroethane in the presence of diisopropylethylamine. The syn/anti selectivity was found be 90%.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-128**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Photocatalytic Oxidation of Benzene to Phenol by Dioxygen with Water as an Electron Source

한지원 이용민[1] 남원우[2,*] Shunichi Fukuzumi[3,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 기초과학연구소 [2]이화여자대학교 화학과 [3]Meijo University

We report herein the efficient photocatalytic hydroxylation of benzene to phenol by dioxygen (O_2) with $[Ru^{II}(Me_2phen)_3]^{2+}$ (Me_2phen = 4,7-dimethyl-1,10-phenanthroline) used as a photocatalyst in the presence of water as an electron source together with $[Co^{III}(Cp^*)(bpy)(H_2O)]^{2+}$ (**1**: Cp* = η^5-pentamethylcyclopentadienyl, bpy = 2,2-bipyridine), which acts as an efficient catalyst for water oxidation as well as benzene hydroxylation to attain TON higher than 400 based on **1**. Photocatalytic hydroxylation of benzene was performed under visible light irradiation in O_2-saturated MeCN-H_2O (*v*/*v* 23:2) mixture solvent containing $Sc(NO_3)_3$ at 298 K. It has been confirmed that the photoexcitation of $[Ru^{II}(Me_2phen)_3]^{2+}$ results in electron transfer from the triplet excited state of $[Ru^{II}(Me_2phen)_3]^{2+}$ to O_2 to produce $[Ru^{III}(Me_2phen)_3]^{3+}$, which can oxidize H_2O to O_2 by catalysis of **1**, and $O_2^{\bullet-}$–Sc^{3+} species by following formation of H_2O_2, which can react with benzene in the presence of **1**. In this presentation, we demonstrate the combination of the photocatalytic H_2O_2 production by H_2O oxidation with O_2 reduction under visible light irradiation and the efficient catalytic hydroxylation of benzene to phenol with H_2O_2 without any malign by-products.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-129**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Production of two dimensional inorganic-organic halide perovskite thin films by spin-coating method

박가람 김기연[1,*] 오인환[2] 박승일[3]

고려대학교 화학과 [1]한국원자력연구원 중성자과학연구부 [2]한국원자력연구소 중성자과학연구부 [3]한국원자력연구원 중성자장치개발관리부

Inorganic-organic halide perovskite type materials attract many scientific interests because of their various application possibilities such as solar cells, thermoelectrics and unique magnetic properties. $(C_6H_5CH_2CH_2NH_3)_2MnCl_4$ (Mn-PEA) and $(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA) belong to the layered inorganic-organic halide perovskite system. These two materials crystallized in the same space group (No. 61, $P\ 2_1/b\ 2_1/c\ 2_1/a$) at room temperature and show the almost same lattice parameters (a = 7.207Å, b = 7.301Å, c = 39.413Å for Mn-PEA, a = 7.187Å, b = 7.344Å, c = 38.549Å for Cu-PEA), the magnetic behaviors are different (antiferromagnetic for Mn-PEA, T_N=43K, ferromagnetic for Cu-PEA, T_C=10K). In this work, we will present the inorganic-organic halide perovskite thin film production process using spin coating method and crystallographic results of Mn-PEA, Cu-PEA and Cu-PEA/Mn-PEA heterostructures using x-ray reflectivity and cross-sectional transmission electron microscopy. Reference

[1] Park et al., Dalton Trans. Vol. 41, 1237 (2012)
[2] Polyakov et al., Chem. Mater. Vol. 24, 133 (2012)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-130**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mononuclear Nonheme High-Spin (*S* = 2) *versus* Intermediate-Spin (*S* = 1)Iron(IV)-Oxo Complexes in Oxidation Reactions

배성희 이용민[1] 남원우[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 기초과학연구소 [2]이화여자대학교 화학과

Mononuclear nonheme high-spin ($S = 2$) iron(IV)-oxo species have been identified as the key intermediates responsible for the C-H bond activation of organic substrates in nonheme iron enzymatic reactions. However, more than 90% of the synthetic nonheme iron(IV)-oxo complexes reported so far possess an intermediate ground spin state ($S = 1$), whereas only a small number of nonheme high-spin (HS) iron(IV)-oxo complexes have been published. Moreover, most of the reactivity and mechanistic studies were conducted using the intermediate-spin (IS) iron(IV)-oxo complexes in nonheme iron models. In contrast, the reactivities of the HS iron(IV)-oxo complexes in oxidation reactions are poorly understood. In this presentation, we demonstrate that the C-H bond activation of hydrocarbons by a synthetic mononuclear nonheme HS iron(IV)-oxo complex occurs through an oxygen non-rebound mechanism, as previously reported in the C-H bond activation by nonheme IS iron(IV)-oxo complexes. We also report that C-H bond activation is preferred over C=C epoxidation in the oxidation of cyclohexene by the nonheme HS and IS iron(IV)-oxo complexes, whereas the C=C double bond epoxidation becomes a preferred pathway in the oxidation of deuterated cyclohexene by the nonheme HS and IS iron(IV)-oxo complexes. In the epoxidation of styrene derivatives, the HS and IS iron(IV)-oxo complexes are found to have similar electrophilic characters.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-131**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of SERS-Active Au Particles Using Furfuryl Alcohol and Furfurylamine As Reducing Agents

김기정 허성*

한국외국어대학교 화학과

Two different types of SERS-active Au microparticles were simply prepared through the redox reaction between Au precursor, $AuCl_4^-$, and furfuryl derivatives without any extra metal surface capping ligands in deionized water at room temperature. Furfuryl alcohol (FA) and furfurylamine (FFA) were used as sole reducing agents for the reduction of Au precursor. Both FA and FFA polymerized during the redox reaction to form polymers. These polymers are thought to act as surface capping ligands during the formation of Au particles. Experiments were proceeded with three different concentrations of each furfuryl derivative. Interestingly, nanoscale Au particles prepared from the reaction with FFA had a large difference in size of the Au particles. The higher concentration of FFA, the smaller the size of Au particles. The size of Au particles was in the range of 1 μm to under 10 nm. Au particles were deposited on a Si wafer by drop-casting and were used as highly active surface-enhanced Raman spectroscopy (SERS) substrates for the detection of methylene blue and crystal violet.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-132**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Allosteric gate opening of folded supramolecular cage

황지은 김영훈[1] 허정석*

충남대학교 화학과 [1]POSTECH 화학과

"Cage" compounds formed by covalent bonds between organic compounds can be designed and prepared in order to possess large cavities. This kind of porous organic solids has been researched for lots of applications such as gas adsorption, catalysis, drug delivery, ion exchange, and sensing. Also, cage can selectively accommodate guest molecules using pore geometry based on 'Host-Guest system'. Especially, the cages synthesized by chiral compounds have a potential for enantioselective recognition. Herein, we report on the synthesis and characterization of a cage molecule using (2,2-Bis(4-hydroxy-3,5-diformylphenyl)propane and enantiopure (1*S*,2*S*)-(+)-1,2-Diaminocyclohexane. The cage structure was characterized by single-crystal X-ray diffraction analysis, revealing the formation of [4+8] cage. Furthermore, we have demonstrated that the cage can individually recognize the enantiomers of mandelic acid, a precursor of many kinds of drugs, by ^{1}H-NMR analyses. Therefore, this cage has a great potential for enantioselective recognition and separation via host-guest interaction. The synthetic scheme and the X-ray structure of the cage and ^{1}H-NMR experiments on chiral recognition will be presented in the poster session. Moreover, metal binding to the cage compound induced transformation of overall structure from folded structure to open cage just like proteins regulates its active site in allosteric manner. Related spectroscopic data will be presented in the poster session. References1. Duff, J. C., J. Chem. Soc, 1934, 282, 13052. Tomokazu Tozawa, Nature materials, 2009, 8, 973-9783. Noriaki Fukuda et al., Tetrahedron: Asymmetry 2009, 20, 111-114

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-133**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of a zinc-homobimetallic catalyst for cycloaddition reactions of CO_2 and epoxides

황지은 허정석*

충남대학교 화학과

To date, carbon dioxide has been considered as a greenhouse gas leading to global warming. Because of this concern, a lot of scientists have researched a variety of applications utilizing carbon dioxide as a kind of sustainable resources. Among the applications, a cycloaddition reaction of CO_2 and epoxides to form useful cyclic carbonates is one of promising researches. Here we report a homobimetallic catalyst for cycloaddition reaction of CO_2 and various epoxides such as propylene oxide, cyclohexene oxide and styrene oxide. The ligand of the catalyst was synthesized by imine-condensation reactions of salicylaldehyde and 2,2-Bis(3-amino-4-hydroxyphenyl)propane. We prepared a Zn-catalyst which has tetradentate coordination by the combination of this ligand and zinc(Ⅱ) acetate. Particularly, the catalyst showed a good catalytic performance of forming styrene carbonates from styrene oxide with approximately quantitative conversion (97.4%) within 24 hours. Details of the work including ^{1}H-NMR spectra, catalytic activity on cycloaddition reactions with various epoxides will be presented in the poster session.References1. Tsumaki, T., Bull. Chem. Soc. Jap., 1938, 13, 252-2602. Jianmin Sun, Green Chem., 2004, 6, 613-6163. Bun Yeoul Lee, J. Am. Chem. Soc. 2005, 127, 3031-3037

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-134**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Slower exergonic electron transfer than direct oxygen atom transfer in the oxidation of triphenylphosphine derivatives by a triflic acid-bound nonheme Mn(IV)-oxo complex

유미 이용민[1] **Shunichi Fukuzumi**[2,*] 남원우[3,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 기초과학연구소 [2]Meijo University [3]이화여자대학교 화학과

Electron-transfer reactions play an important role in chemical and biological systems. When electron transfer is exergonic and energetically feasible, electron transfer generally occurs first prior to bond cleavage and formation, because little interaction is required for electron transfer occur at the relatively long distance. The mechanism is changed from two-electron processes including bond cleavage and formation to electron transfer to be the rate-determining when the redox potentials are changed in favor of electron transfer. In this presentation, exergonic electron transfer from triphenylphosphine (PPh_3) derivatives to a triflic acid (HOTf)-bound nonheme Mn^{IV}-oxo complex, $[Mn^{IV}(O)]^{2+}$-$(HOTf)_2$, is slower than direct oxygen atom transfer from $[Mn^{IV}(O)]^{2+}$-$(HOTf)_2$ to PPh_3 derivatives because of the large reorganization energy of electron transfer, in contrast with much faster electron transfer from thioanisole derivatives to $[Mn^{IV}(O)]^{2+}$-$(HOTf)_2$ than the direct oxygen atom transfer.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-135**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of Cu(II) complexes bearing dichloro benzyl and o-methoxy benzyl derivate of (R,R)-1,2-diaminocyclohexane and its application toward Asymmetric Nitroaldol reaction

조주현 정종화*

경북대학교 화학과

Homo-chiral Cu(II) complexe with N-2-methoxybenzyl -N’-2,6-dichlorobenzyl-(R,R)-1,2-diaminocyclohexane (MDAC) ligand was synthesized and characterised. The X-ray crystal structure of Cu(II) complex containing MDAC was determined. (S, R)(1R,2R) and (R, S)(1R,2R)-coordination complexes were cocrystallized. The geometry around the Cu(II) centre for (MDAC)CuCl2 was distorted square-pyramidal. A strong interaction between the Cu and O of the methoxy group. Catalytic activities of diacetato Cu(II) complex with 10 mol% of diisopropylethylamine in the asymmetric Henry reaction of bezaldehyde and nitro-mthane or nitro-ethane were examined.

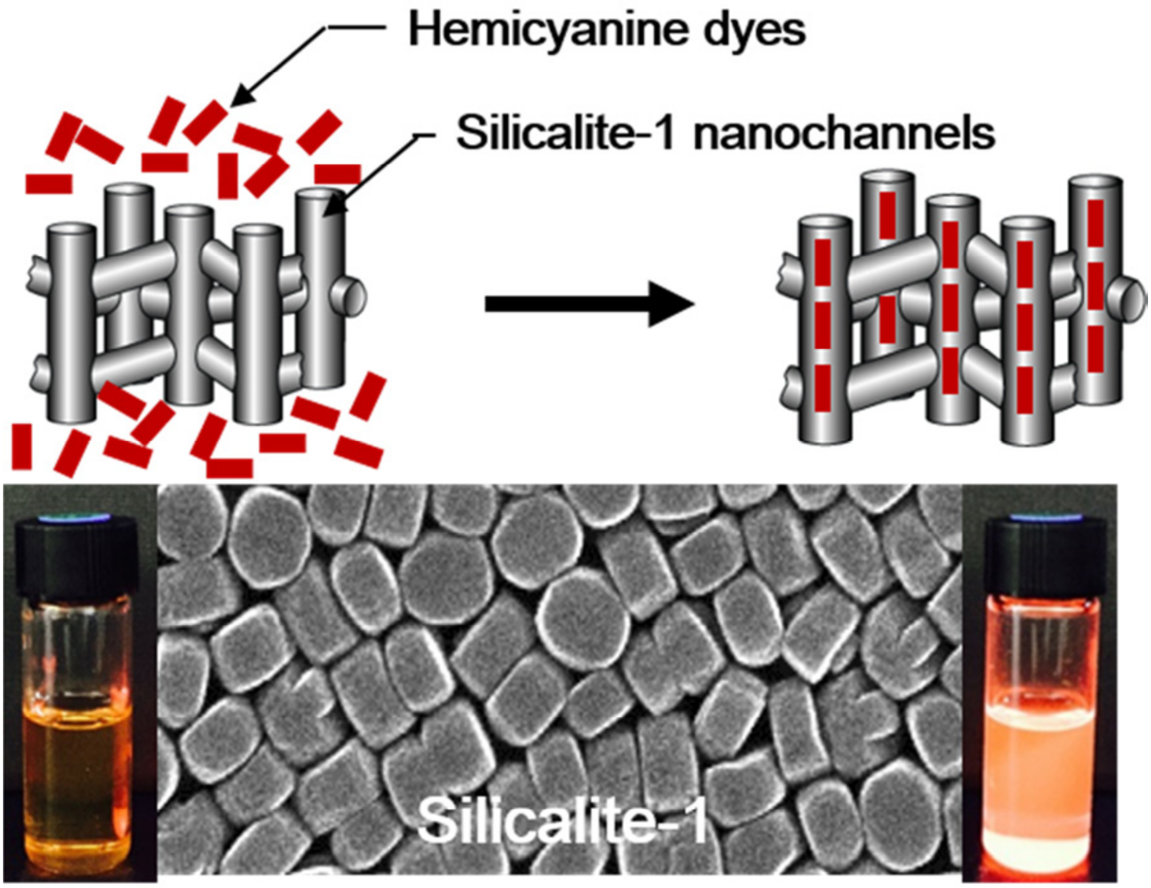
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-136**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhancement of fluorescence from one- and two-photon absorption of hemicyanine dyes by confinement in silicalite-1 nanochannels

김현성* <u>김다인</u>

부경대학교 화학과

We have prepared a unique, organic–inorganic composite having strong one- and two-photon florescence properties by encapsulating hemicyanine molecules in nanosized silicalite-1 zeolite. The isolation and confinement of the hemicyanine dramatically enhances its fluorescence from one- and two-photon absorption in different solvents. We believe that this study represents a promising new strategy in the development of one- and two-photon fluorescence materials and a promising new direction for zeolite research and its application in the development of optical materials.


Hemicyanine dyes
Silicalite-1 nanochannels
Silicalite-1

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-137**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Activation of C-H bonds over faujasite-type zeolites encapsulated metal-phthalocyanine

김현성* 유혜진

부경대학교 화학과

Metal-phtalocyanine (MPc) complex is widely accepted to be oxidation catalysts for aliphatic C-H bonds in alkanes, alcohols, olefins, aromatic C-H bonds. We have synthesized metal-phthalocyanine containing various type of transition metals such as iron, cobalt and cupper in the supercages of faujasite-type zeolites via “ship-in-a-bottle” procedure. Prepared metal-phthalocyanine zeolites composite was shown to be higher oxidative catalytic activity than the authentic homogeneous catalysts under reaction conditions. Herein, cyclohexane was selectively oxidized to cyclohexanol and cyclohexanone through metal-phthalocyanine zeolite using hydrogen peroxide as oxidant. We also evaluated the type of counter cation of the zeolite framework on the catalytic efficiencies.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-138**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation and Characterization of Porphyrin-Imbedded Silica Aerogels

조민경 김남길 김희준*

금오공과대학교 응용화학과

Silica aerogels are unique materials with extraordinary properties such as high porosity, large surface area, and low refractive indices. Due to these properties, they can be applied to a wide range of areas including, insulation, catalyst support, sensors, and dielectric materials. On the other hand, porphyrins and metalloporphyrins are attracting molecules exhibiting promising photochemical and electrochemical properties in various areas including catalysis, solar energy conversion, and medical application. We have prepared and characterized a new nanomaterials such as tin(IV) porphyrin-imbedded silica aerogels, and will here present in detail.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-139**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Intermetal Oxygen Atom Transfer Reaction from a Mononuclear Iron(V)-Oxo Complex to a Manganese(III) Complex

장수정 홍승우[1] 남원우[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학나노과학부 [2]이화여자대학교 화학과

High-valent iron-oxo intermediates driven catalytic oxidation of organic substrates are of central interest due to their reactivities in versatile biological oxidation reactions. Among the diverse oxidation reactions, the direct oxygen atom transfer (OAT) reactions between an electrophilic terminal oxo moiety and organic substrates. However, the intermetal OAT reaction between a mononuclear nonheme iron(V)-oxo and manganese(III) complex supported by same ligand system has yet been investigated due to the scarcity of iron- and manganese-oxo complexes in +5 oxidation state. In this study, we investigated the direct OAT reaction between the iron(V)-oxo complex and the manganese(III) complex supported by identical tetraanionic tetraamidomacrocyclic ligand (TAML) that resulted in the formation of a manganese(V)-oxo complex.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-140**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structure, Synthesis and Characterization of Bis(diamino-diamido)-tetrathiafulvalene

KhanMohammadSherjeelJaved 조장훈 이홍인*

경북대학교 화학과

In the past decades, one of the massive demand in the tetrathiafulvalene (TTF) field has been to assemble new bifunctional TTF derivatives in which the redox functional TTF part is combined with other functional groups. Redox systems of TTF-derivatives have received extensive attention for applications in ion sensors and supramolecular devices. The redox-dependent proton translocation is very important and useful in bio systems, and has been studied for molecular sensors. For the amido-TTFs, scientists concentrate their importance on the crystal engineering of hydrogen-bond association but only an insufficient research have been accomplished on the bifunctional application in redox recognition. The amido group can form strong hydrogen bonds and become one of the utmost popular hydrogen-bond donors used in ion sensors We have lately designed a new TTF derivative with the diamino-diamido group, bis(diamino-diamido)- tetrathiafulvalene (TTF(CONHCH2CH2NH2)4. The new compound has two sets of diamino-diamido groups on symmetric sides and it is conventional that the compound could add new properties to TTF-diamino-diamido derivatives.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-141**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Structural studies of Nickel complexes ofN,N'-Disalicylidene-2,2'-(ethylenedioxy)bis(ethylamine)

임종완

심인고등학교 화학

Two nickel complexes [Ni(L)2CH3OH](CH3OH)2, [Ni(L)2O] [L=N,N'-Disalicylidene-2,2'-(ethylenedioxy)bis(ethylamine)] have been prepared and characterized by X-ray diffraction measurements. The crystallographic analysis of the complex revealed that the two nickel complexes are dinuclear structure.

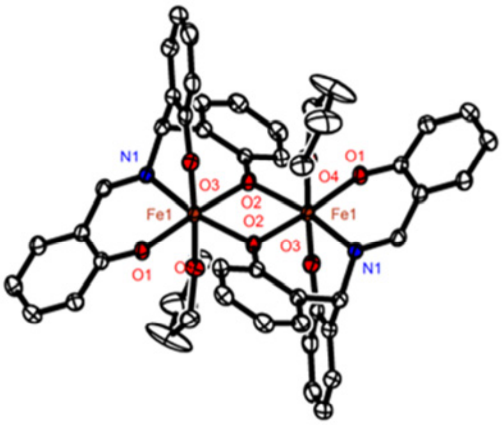
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-142**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Iron Catalysts for the Coupling Reaction of CO_2 and Epoxides

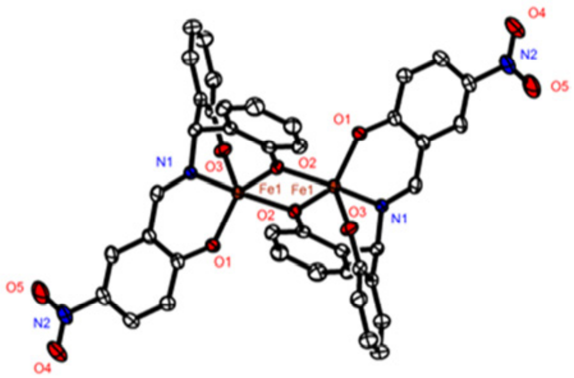
이다영 이윤호*

KAIST 화학과

Carbon dioxide conversion into valuable chemicals has received much attention since it has potential applications as an abundant, nontoxic and renewable C1 source. The most widely studied area in the activation of CO_2 is its coupling reaction with various epoxides to produce industrially important commodity chemicals such as, polycarbonate and cyclic carbonate. Cyclic carbonates have potential applications in various industries as the precursors for polycarbonate, solvents of electrolyte and intermediates of organic synthesis. In order to work with the selective and effective conversion of CO_2 to cyclic carbonate, we have designed a new ligand scaffold that can accommodate an iron center in a three fold symmetry. Specifically, we are designing a new catalyst based on understanding the relationship between the metal's geometry and its catalytic activity. Two iron complexes, $\{(NO_3)Fe(THF)\}_2$ (Fe-1a) and $\{[(5\text{-}NO_2)NO_3]Fe\}_2$ (Fe-1b), were synthesized and well characterized by various spectroscopic techniques and X-ray crystallography. Solid-state structures reveal the dimeric nature of Fe-1a and Fe-1b where the available binding sites for each metal center are occupied by bridging phenolate oxygen atoms. In order to achieve the high catalytic performance with Fe-1a, reaction conditions were optimized with several variables including pressure, temperature and co-catalyst/catalyst ratio. Under the optimized conditions, Fe-1a showed unusual catalytic efficiency with propylene oxide. Detailed characterization and catalytic reaction will be presented.


N1
O3
O2
O4
O1
Fe1
O2
Fe1
O1
O3
N1
O3

Fe-1a


O4
N2
O5
O1
N1
O3
O2
Fe1
Fe1
O2
O3
N1
O1
O5
N2
O4

Fe-1b

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-143**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of a New Polar Titanium-Organic Coordination Polymer

김봉수 옥강민*

중앙대학교 화학과

A novel polar noncentrosymmetric (NCS) titanium-organic coordination polymer has been synthesized by a solvothermal reaction at 130 °C using titanium isopropoxide, pyridinedicarboxylic acid, piconilic acid, and dimethylammonium iodide. The crystal structure of the reported material has been determined by single-crystal X-ray diffraction. The material has an anionic one-dimensional framework composed of seven-coordinate titanium, pyridinedicarboxylate, and picolinate groups. Powder second-harmonic generating (SHG) measurements on the polycrystalline sample of the reported material indicate that the compound exhibits SHG efficiency of 400 times that of • •SiO2 and is phase-matchable (type-1). The material also reveals a very interesting water molecule-driven reversible phase transition .Further detailed structural analysis and characterizations including SEM/EDAX, IR and UV−Vis diffuse reflectance spectroscopies, thermogravimetric analysis, and elemental analysis will also be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-144**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optical Properties for New Noncentrosymmetric Sodium Lanthanide Iodates, NaLn(IO3)4 (Ln = La, Ce, Sm, and Eu)

오승진 김형구 옥강민*

중앙대학교 화학과

Crystals of four isostructural iodates, NaLn(IO3)4 (Ln = La, Ce, Sm, and Eu), have been synthesized through hydrothermal reactions. The single-crystal X-ray diffraction reveals that the materials crystalize in the acentric monoclinic space group, Cc (No. 9). The crystals have two-dimensional structures where the sheets are parallel along the a-axis. The layers consist of lanthanide cations coordinated by eight-O atoms of iodate groups leading to anionic frameworks. The Na+ cations act as intra-layer cations to balance the anionic frameworks of the eight-membered-ring channels directed to the (010) plane. Close structure investigation suggests that since the constructive sum of the dipole moments of iodates, the compounds reveal type-I phase matching behavior with strong second harmonic generation (SHG) efficiency of ca. 500 times that of α-SiO2. In addition, photoluminescence (PL) properties were also investigated for Eu-compounds and Ce3+, Sm3+ and Eu3+ doped-NaLa(IO3)4 at various temperatures. The phenomenon that the transition of electric dipole is stronger than that of magnetic dipole was observed in the PL emission spectra for Sm3+ and Eu3+, which confirms that the environment of the materials is asymmetric. Infrared, UV-vis spectroscopy, thermal analyses, and their dipole moment calculations are also investigated.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-145**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

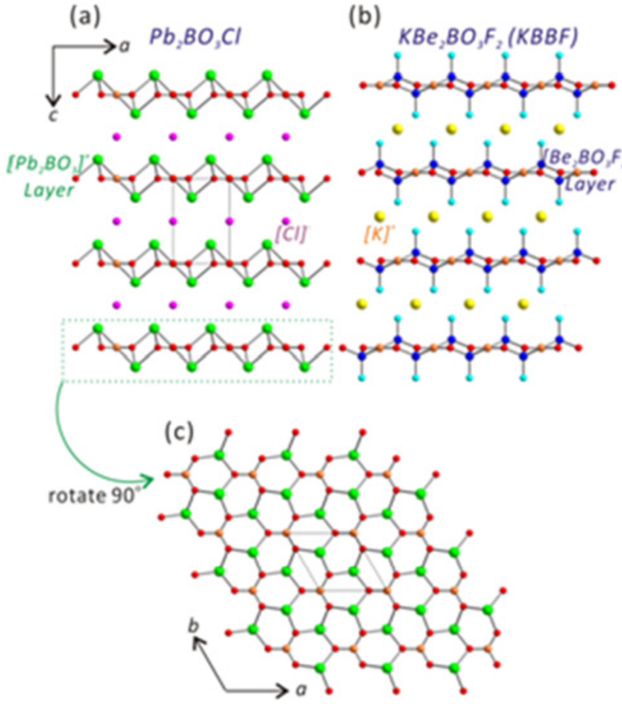
Pb_2BO_3Cl: A New Tailor-Made Polar Lead Borate Chloride Exhibiting Very Strong Second-Harmonic Generation Response

Zouguohong 옥강민*

중앙대학교 화학과

Nonlinear optical (NLO) materials, the key components for solid state lasers producing coherent light through a cascaded frequency conversion, have drawn extensive commercial and academic interests attributed to their versatile scientific and technological applications. In the past several decades, many efforts have been made to elucidate the inter-relationships of the structures, compositions, and NLO properties of the crystalline compounds; however, it still remains challenging to efficiently design novel NLO materials with excellent comprehensive properties including large second-harmonic generation (SHG) coefficients, moderate birefringence for the phase-matching condition, wide transparency windows for the high damage threshold, good chemical stability, and facile crystal growth, etc.

In this research, a meticulously designed novel polar noncentrosymmetric (NCS) lead borate chloride, Pb_2BO_3Cl was successfully synthesized through a molecular engineering approach using $KBe_2BO_3F_2$ (KBBF) as a model. Single-crystal X-ray diffraction revealed that the structure of Pb_2BO_3Cl consists of very interesting cationic $[Pb_2(BO_3)]^+$ honeycomb layers and Cl^- anions. The powder second-harmonic generation (SHG) measurements on the graded polycrystalline Pb_2BO_3Cl indicated that the title compound is phase-matchable (type I) and exhibits a remarkably strong SHG response of approximately 9.0 times that of potassium dihydrogen phosphate (KDP), which is the largest efficiency observed in the materials containing similar structures with KBBF. Further characterization suggested that the reported compound melts congruently at high temperature and has a wide transparency window from the near-UV to mid-IR region.


(a)
Pb2BO3Cl
a
c
[Pb2BO3]+
Layer
[Cl]-
(b)
KBe2BO3F2 (KBBF)
[Be2BO3F2]-
Layer
[K]+
(c)
rotate 90°
b
a

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-146**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

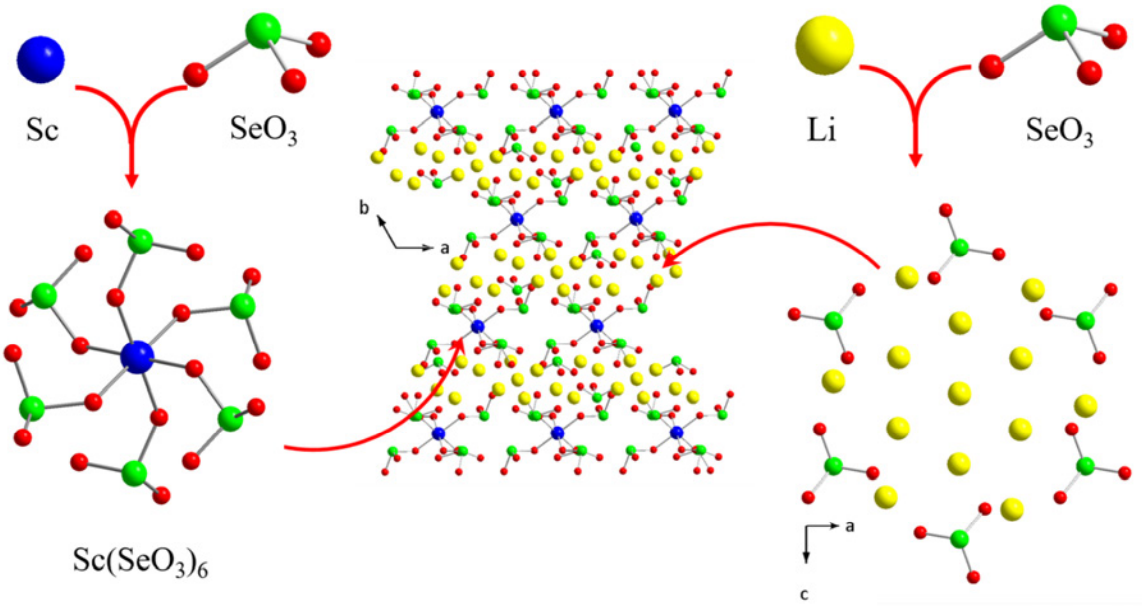
Synthesis, structure determination, and characterization of a new lithium scandium selenite

조홍일 송승윤 옥강민*

중앙대학교 화학과

A new lithium scandium selenite was synthesized by hydrothermal and solid state reactions using Li_2CO_3, Sc_2O_3, and SeO_2 as reagents. The crystal structure of the newly synthesized selenite was determined by single crystal X-ray diffraction. The lithium scandium selenium oxidereveals a molecular structure consisting of ScO_6octahedra, SeO_3 trigonal pyramids, and Li^+ ion.

Infrared spectrum indicates Se-O and Sc-O vibrations at ca. 600-900 $cm^{-1}$and 450-580 cm^{-1}, respectively. The band gap calculated by Kubelka-Munk function using the UV-vis diffuse reflectance spectrum of the selenite is about 4.94 eV.Thermogravimetric analysis of the selenite suggests that the material is thermally stable up to 560 ℃.
Detailed structural analysis along with dipole moment calculations will be presented.


Sc
SeO_3
Li
SeO_3
b
a
$Sc(SeO_3)_6$
a
c

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-147**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel phenanthroimizole based *N*-phenyl or biphenyl triarylborane; intriguing “turn-on” emission upon binding fluoride anion

유동균 이선희[1] 박명환[1,*] 이강문[*]

강원대학교 화학과 [1]충북대학교 화학교육과

The four kinds of novel *N*-Triarylborane-phenanthroimidazole complexes bridged by a biphenylene or phenylene group were prepared and characterized by multinuclear NMR spectrum and elemental analysis. All of the complexes show highly fluorescent property, positive solvatochromism and the moderate fluoride binding ability. Especially, Upon fluoride binding to the boron center, they exhibit a ratiometric fluorescence response accompanying a turn-on emissive band, resulting in vivid emission color change. These specifically photophysical characters were also studied with TD-DFT calculations. Consequently, these complexes can be utilized as the efficient turn-on chemosensors for a fluoride anion.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-148**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel dimeric *o*-carboranyl triarylborane ratiometric color-tunable sensor and its theoretical studies

최병훈 박명환[1,*] 이강문[*]

강원대학교 화학과 [1]충북대학교 화학교육과

A dimeric *o*-carboranyl triarylborane compound (2) with a biphenylene bridge group was prepared and characterized. Also, its solidstate structure was determined via X-ray diffraction. Treatment of 2 with an excess amount of KF in the presence of 18-crown-6 formed a dimertypepotassium salt, $[2\cdot F_2][K\cdot 18\text{-crown-6}]_2$; its structure was fully confirmed by multinuclear NMR spectroscopy. UV−vis titration experiments carried out in THF showed that 2 binds fluoride ions witha binding constant (K) of 8.5×10^5 M^{-1}. The linear decline of the UV/visabsorption of 2 upon titration with fluoride suggested that the triarylborane moieties acted as independent binding sites, which were not affected by each other. Contrary to a single emission (λ_{em} = 376 nm) of 2 assignable to an intramolecular charge transfer (ICT) transition at 298 K in THF, a broad low-energy emission band was additionally observed at 77 K, which is dominant in the film state. The TD-DFT calculation on the first excited singlet state of 2 shows that the low-energy emission band originates from the CT nature between carborane and triarylborane groups. Aggregation-induced emission (AIE) of 2 was clearly confirmed by enhanced photoluminescence intensity (λ_{em} = 489 nm) upon increasing the water fraction (f_w) in the THF solution of 2, and it further accounts for the intense emission in the solid state. Interestingly, the emission spectrum of a film sample of 2 upon addition of two equivalents of fluoride ion was was mostly similar to that of $[2\cdot F_2][K\cdot 18\text{-crown-6}]_2$, indicating that the ICT-based AIE nature of 2 could be red-shifted by fluoride binding.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-149**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Scavenging Roles of Trimetallacyclophanes in Photo-cyclopropanation Reactions

이해리 정옥상*

부산대학교 화학과

The palladium(II)cyclophane systems, constructed by previously reported proof-of-concept self-assembly, represent a crucial landmark in the field of effective and recyclable scavenging 6 equiv. of triiodide (I_3^-) per 1 equiv. of scavenger in photo-cyclopropanation of alkenes with CH_2I_2. The scavenger's driving force behind photo-cyclopropanation is the efficient *in situ* crystallization of triiodide-exchanged species. The exact quantitative photoreaction yields according to the mole ratios of the cyclophane system are impressive. The recycling behavior can be ascribed to the rigidity and stability of the four-layered tripalladium(II)cyclophane.

Reference
[1] Lee, H.; Noh, T. H.; Jung. O.-S. *Angew. Chem. Int. Ed.* **2016**, *55*, 1005.
[2] Lee, H.; Choi, E.; Noh, T. H.; Jung. O.-S. *Dalton Trans.* **2016**, *submitted*.

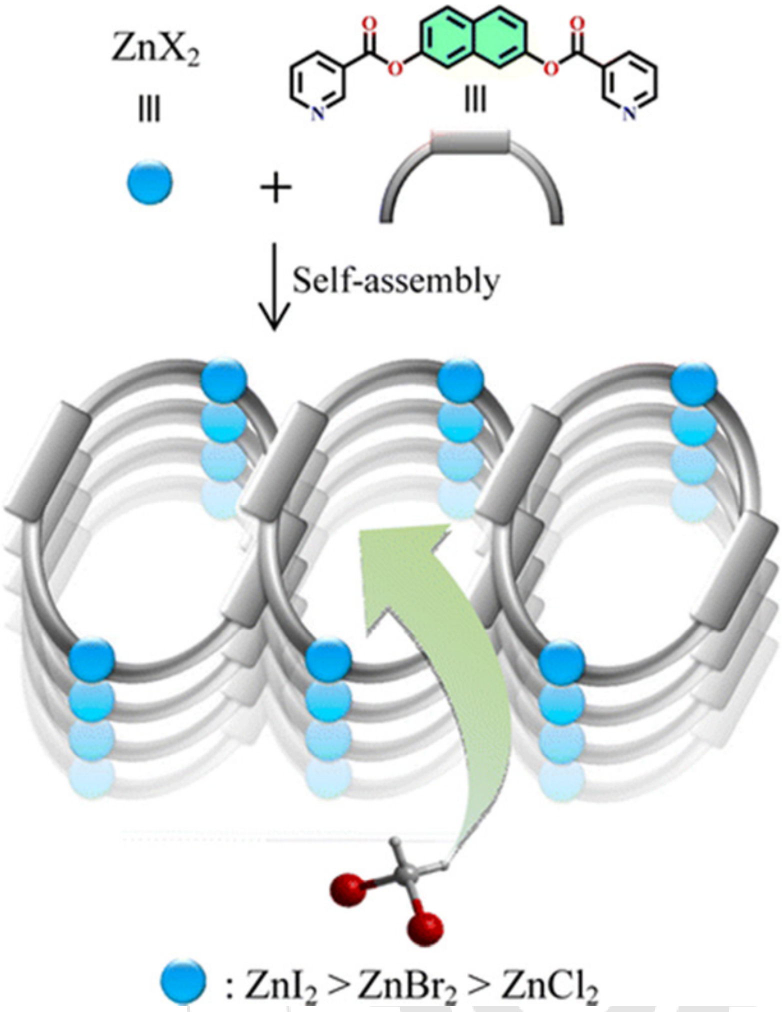
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-150**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Host-Guest Chemistry of 1D Suprachannels Consisting of Cyclodimeric Zn(II) Complexes

류민주 정옥상*

부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with 2,7-bis(nicotinoyloxy)naphthalene (L) as a hemicircular bidentate ligand containing a chromophore moiety yields a systematic metallacyclodimeric unit, $[ZnX_2(L)]_2$. These basic skeletons constitute, via interdigitated $\pi\cdots\pi$ interactions, a unique columnar ensemble forming a suprachannel. This can then be employed as an unusual “diiodomethane within the suprachannel” host-guest system, $CH_2I_2@[ZnX_2(L)]_2$. Specifically, the suprachannel significantly stabilizes the CH_2I_2 molecules in the order $[ZnI_2(L)]_2 > [ZnBr_2(L)]_2 > [ZnCl_2(L)]_2$. This suprachannel has significant halogen effects on the photoluminescence(PL), thermal properties, and host-guest inclusion.Scheme 1. Schematic Diagram for the Present ComplexesReference. [1] Park, M.; Kim, H.; Lee, H.; Noh, T. H.; Jung, O.-S. *Cryst. Growth Des*. 2014, *14*, 4461-4467.


ZnX$_2$
O
O
N
O
O
N
+
Self-assembly
● : ZnI$_2$ > ZnBr$_2$ > ZnCl$_2$

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-151**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation and Physicochemical Properties ofMercury(II) Complexes Depending on Halide Anions

황서영 정옥상*

부산대학교 화학과

Self-assembly of HgX_2 (X^- = Cl^-, Br^-, and I^-) with Y-type 2,6-bis[(2-isonicotinoyloxy-5-methylphenyl)methyl]-1-isonicotinoyloxy-4-methylbenzene (L) yields 2D consisting of alternate prismatic P- and Mhelical-linked-layers, 1D consisting of P- and M-helices, and simple 2D sheet in a unique Y-type mode, respectively. The L/Hg(II) ratio of each product (3/3 for Cl^-; 2/3 for Br^-; 1/3 for I^-) is dependent on the nature of the halide anions. The coordinating environments around of Hg(II) ion approximate to a square pyramid for Cl^-, a square planar and a distorted tetrahedral geometry for Br^-, and distorted tetrahedral arrangement for I^-, respectively. Photoluminescence wavelengths are strongly depending on the halide anions, and coordination ability to L is in the order of X^- = Cl^- > Br^- > I^-. Such physicochemical properties were explained by electronic and steric natures of halide anions. Reference [1] Choi, E.; Kwon, N.; Kim, J. G.; Jung. O.-S.; Lee, Y.-A. *J. Mol. Struct.* 2016, *1118,* 367-370

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-152**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Construction of 1D Silver(I) Coordination Polymers Consisting of Y-type Tridentate Ligands

최다예 정옥상*

부산대학교 화학과

Dimensionality of metal-organic coordination polymers plays a key role in determination of their task-specific functions. Their dimensions have been generally driven by a suitable combination of the coordination geometry of metal center and the donor-numbers of linkers or by unpredictable weak interactions. In particular, 1D skeleton is one of the simplest practical polymeric arrays including chains, loops, helices, and spiro-links which are useful to gas adsorption, mixed-valence system, photo-induced electron or energy transfer, magnetic exchange, semiconductors, catalysts, luminescent chemosensors, and ion-exchangers. Thus, construction of desirable motif 1D coordination polymers via delicate manipulation of some reaction-components is a challengeable work in the field of supramolecular materials. Various motif 1D coordination polymers containing designed interesting bidentate ligands have been formed, but the systematic 1D coordination polymers containing *o*-, *m*-, and *p*-tridentate ligands are relatively rare. To date, such tridentate ligands have been usually employed for generating coordination cages or triangular module metal complexes for the past decade.Self-assembly of silver(I) hexafluorophosphate with unique Y-type tridentate ligands (2,6-bis[(2-picolinoyloxy-5-methylphenyl)methyl]-*p*-tolylpicolinate (*o*-L), ***2-nicotinoyloxy-*** (*m*-L), and ***2-isonicotinoyloxy-*** (*p*-L)) produces single crystals consisting of 1D loop-and-chain coordination polymers of $[Ag(o\text{-}L)](PF_6)\cdot Me_2CO\cdot CHCl_3$, $[Ag(m\text{-}L)](PF_6)\cdot Me_2CO$, and $[Ag_3\ (p\text{-}L)_2](PF_6)_3\cdot 2H_2O\cdot 2C_2H_5OH\cdot 4CH_2Cl_2$ with quite different trigonal prismatic, trigonal, and linear silver(I) coordination geometry, respectively. Coordinating ability of the three ligands for $AgPF_6$ is in the order of *p*-L > *o*-L > *m*-L. The solvate molecules of $[Ag(o\text{-}L)](PF_6)\cdot Me_2CO\cdot CHCl_3$ can be removed, and be replaced reversibly in the order of acetone > chloroform ≈ dichloromethane >> benzene, without destruction of its skeleton..

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-153**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Catalytic Efficiency of As-synthesized Cyclodimeric Cu(II) complexes depending on Steric Hindrance of both Catalysts and Substrates

이상석 정옥상*

부산대학교 화학과

Catechol oxidases are omnipresent type III dicopper-active site enzymes that catalyze the aerial oxidation of versatile catechol species to the corresponding *o*-quinones along with the reduction of oxygen to water. The catechol oxidation reaction is of considerable importance to medical diagnosis of hormonally active catecholamines such as adrenaline, noradrenaline, and 3,4-dihydroxyphenylalanin. Thus, desirable synthesis and catalysis of unique dicopper analogues have been hot issues in the bioinorganic field for the two decades. Some dicopper complexes have shown considerably effective activity according to the nature of bridging coligands, ligands, electrochemical potentials, and *p*H. The number and structure of bridging coligands between the copper centers in a dicopper complex are particularly significant factors in the catechol oxidation catalysis.Reaction of CuX_2 with new ligand, 1,4-bis(dimethyl(quinolin-3-yl)silyl)benzene (L), in alcohol affords C_2-symmetric double-alkoxy-supported cyclodimeric copper(II) complexes, $[Cu(\mu\text{-}OR)(L)]_2(X)_2$ (R = Me, Et, ^{i}Pr; $X^- = ClO_4^-, BF_4^-$) in high yields. These cyclodimeric species with intracyclic Cu···Cu distances of 2.92–2.98 Å show the significant catalytic effects on the catechol oxidation catalysis in chloroform in the order $[Cu(\mu\text{-}OMe)(L)]_2(X)_2 > [Cu(\mu\text{-}OEt)(L)]_2(X)_2 > [Cu(\mu\text{-}O^iPr)(L)]_2(X)_2$. Furthermore, the catalytic efficiency is strongly substrate-dependent in the order 4-BuCat > 4-ClCat > 3,5-DBuCat > Cat. Such notable catalytic effects potentially can be explained by the steric hindrance of both catalysts and substrates.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-154**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Unprecedented Chloride-bridged-bis(halo)mercury(ll) Complexes via *in situ* Crystallization under UV-irradiation in Chloroform Media

최은경 정옥상*

부산대학교 화학과

Self-assembly of HgX_2 ($X^- = Br^-$ and I^-) with new 1,1,2,2-tetramethyl-1,2-di(pyridin-3-yl)disilane (L) ligand affords single crystals consisting of sinusoidal-strand coordination polymers, $[HgX_2L]$. Specifically, 350 nm UV irradiation of crystalline products $[HgBr_2L]$ and $[HgI_2L]$ in chloroform media forms *in situ* single crystals of extraordinary chloro-bridged mercury species, $[H_2L]^{+2}[Hg_2Br_4(\mu\text{-}Br)(\mu\text{-}Cl)]^{-2}$ and $[H_2L]^{+2}[HgI_2(\mu\text{-}Cl)]_2^{-2}$, respectively, in high yields that cannot be synthesized by general synthetic procedures. For all of the compounds, the coordination geometries around the Hg(II) ions along with the mechanistic aspects of the formation of chloro-bridged species are discussed herein.Reference [1] E. Choi, H. Lee, T. H. Noh and O.-S. Jung, CrystEngComm 2016 accepted (Front cover)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-155**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

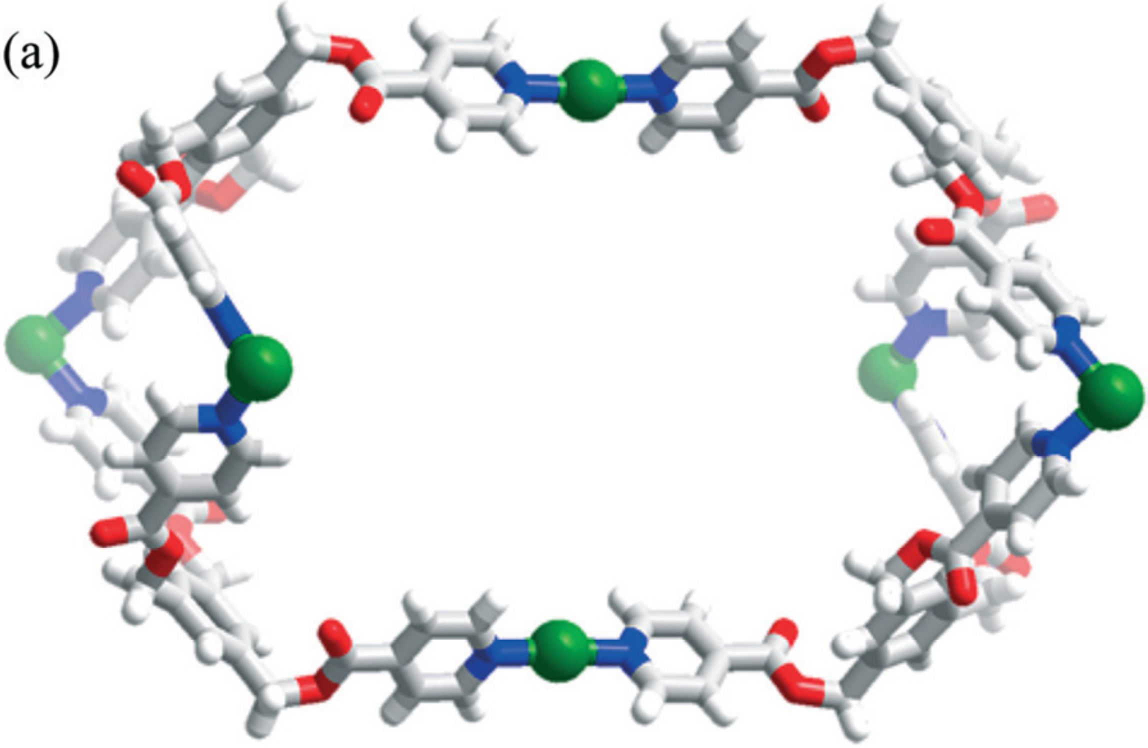
Catalyfic Properties and Solvent Adsorption of Porous Copper(II) Coordination Polymers

이정준 정옥상*

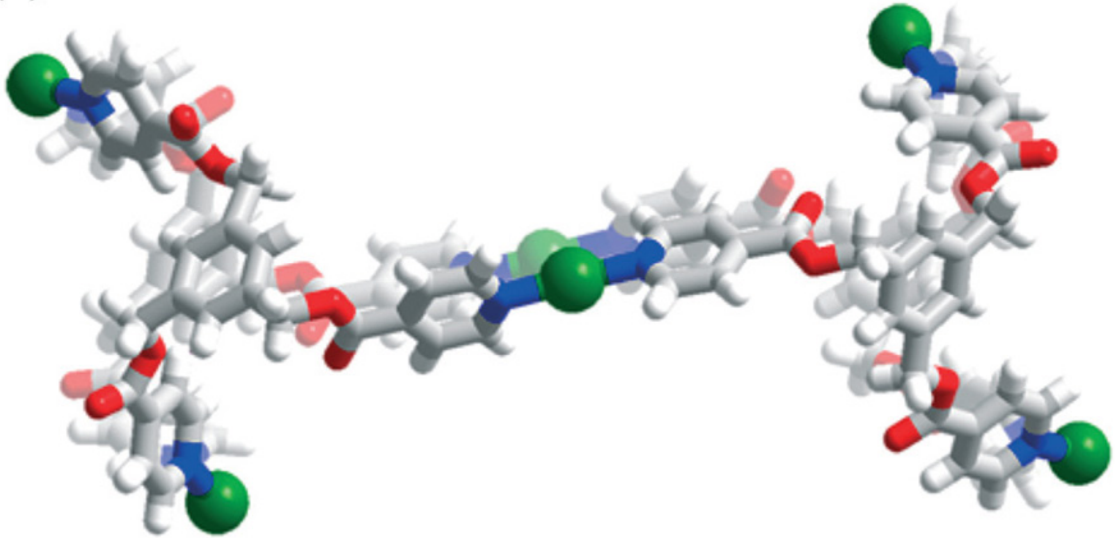
부산대학교 화학과

The reaction of CuX2 (X• •= ClO4• •and BF4•) with a new 1,3,5-tris(isonicotinoyloxymethyl)benzene (L) ligand gives rise to 3D coordination networks, [Cu3L4(CH3CN) 6](X) 6, with a new topology of the Schla¨fli point symbol {4·8• }4{4• •8• •10• }2{8• •12• }. [Cu3L4(CH3CN) 6](ClO4) 6 and [Cu3L4(CH3CN) 6]IJBF4) 6 networks have useful oval-shaped pores of 11.2 × 11.2 × 24.8 Å3 and 11.1 × 11.1 × 24.4 Å3 dimensions, respectively. These porous coordination networks act as good heterogeneous catalysts, oxidizing the catechols in the order 3,5-ditert-butylcatechol (3,5-DBuCat) > 4-tert-butylcatechol (4-BuCat) > 4-chlorocatechol (4-ClCat). The catalytic effect of [Cu3L4(CH3CN) 6](BF4) 6 is slightly higher than that of [Cu3L4(CH3CN) 6](ClO4) 6. The pores of the 3D networks reversibly adsorb the solvents in the order chloroform > tetrahydrofuran > acetone.Figure 1. Side (a) and top (b) views showing the unit cage of [Cu3L4(CH3CN)6](ClO4)6Reference[1] Kim, D.; Kim, B.; Noh, T. H.; Jung. O.-S. CryEngComm 2015, 17, 2583-2590.

(a)



(b)



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-156**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on CO_2 sorption behavior in the functionalized porous coordination polymer

신종원 문도현[1,*]

한국과학기술정보연구원 대구경북지원 [1]포항가속기연구소 빔라인운영부 생명화학소재팀

The functionalized porous coordination polymers (PCPs) or metal organic frameworks (MOFs) have been attracted much attention in material science and chemical industry, because of their versatile applications such as homo/heterogeneous catalyst, molecular recognition of chiral enantiomers and gas storage. Moreover, the well-defined channels in the PCPs or MOFs have definite advantages of the uptake of gas molecules, *i.e.* CO_2, CH_4, N_2 and H_2 gases, and can show high selectivity for guest molecules. These properties in PCPs or MOFs have been widely studied, however, the studies of the behaviors related to the gas/guest molecules in PCPs or MOFs are still rare to find. Recently, a porous coordination polymer, $[(tpmd)Mn(NCBH_3)_2]_n$•x guest (**1**) , was synthesized by the self-assembly of Mn(II) species, $NCBH_3$ anions and *N*,*N*,*N′*,*N′*-tetra-4-pyridyl-methylenediamine (tpmd). To investigate the behaviors of gas molecules in **1**, CO_2 gases were loaded into the dried crystal of **1**, and then, single crystal X-ray diffraction data of **1** were collected and analyzed. The CO_2 molecules in **1** are well located within the channels. Here, we will explain the crystal structure, gas sorption properties and breakthrough data as well as interesting coordination chemistry.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-157**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Current status of the Supramolecular Crystallography Beamline at pohang light source

김대웅 신종원[1] 문도현[2,*]

경북대학교 화학과 [1]한국과학기술정보연구원 대구경북지원 [2]포항가속기연구소 빔라인운영부 생명화학소재팀

포항가속기연구소의 초분자 결정학 빔라인(Supramolecular Crystallography Beamline; BL2D-SMC)은 단결정 회절 분석을 통한 유기, 무기, 무기-유기 혼성 물질의 구조를 분석하고 확인할 수 있는 국내 유일의 방사광 결정학 시설이다. 일반적인 실험실 장치 보다 매우 강력한 방사광 빛을 이용하여 빠른 시간 데이터 수집이 가능하며, 시료 위치에서의 작은 빛의 크기 (100 µm(가로) × 85 µm(수직)) 를 이용하여 매우 작은 단결정 시료의 정확한 구조분석을 할 수 있다. 또한 다양한 영역의 X-선 파장을 선택적으로 사용이 가능하며, 자체 개발된 소프트웨어를 이용하여 쉽게 이용자가 원하는 파장으로 변경하여 실험 및 데이터 수집을 할 수 있다. 최근, 단결정 실험에서 요구되는 다양한 외부자극 (빛, 온도, 기체 흡착 등)을 가한 후 in-situ 로 구조적 변화를 측정하고 분석 할 수 있는 연구를 할 수 있다. 이 포스터를 통하여, 포항가속기연구소의 초분자 결정학 빔라인을 소개하고 관련 실험 장치를 소개하고자 한다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-158**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Nanocrystalline metal-organic frameworks (MOFs) embedded in the other MOF crystals

최경민

숙명여자대학교 화공생명공학부

Design and synthesis of crystalline nanoporous frameworks are usually originated from combining different constituents into the underlying matrix and making them have functions for unique properties. For example, a metal-organic framework (MOF) uses the specific organic linker and metal oxide units to give its unique crystalline and porous structure, while modification by a different organic linker or inorganic moiety can tune the underlying MOF structure to have its other property. This hierarchy allows a facile control in the structure and its property, but some challenges still exist when one pursues the goal to develop a simple method for multifunctional properties without synthesis of the undesirable complex structure. Here, we report a new method to combine completely different MOFs together in a single body. This method opens many opportunities to formation for a series of the heterogeneity in the ordered other MOF embedding the nanocrystals of a MOF (nMOF) with the special constructions and micropores.

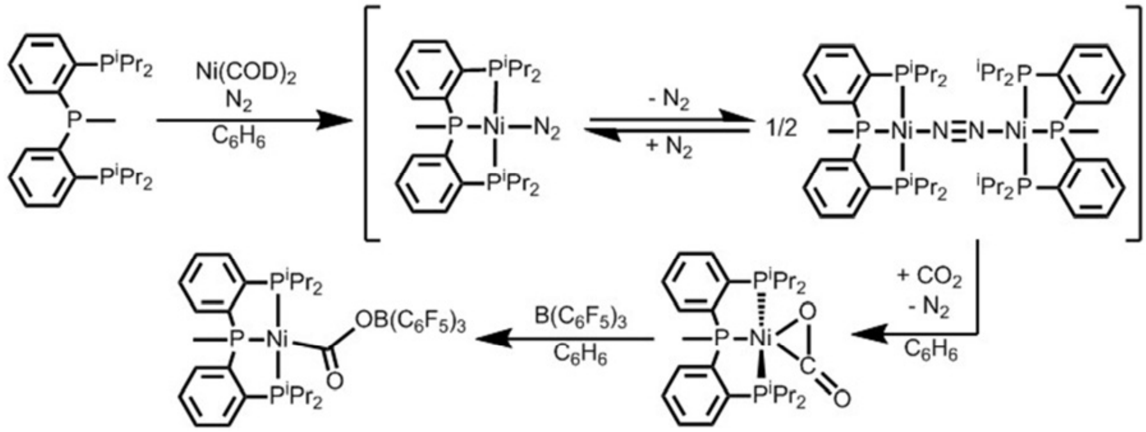
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-159**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Transformation of Carbon Dioxide Inspired by CODH Active Site

김동언 김영은 이윤호[*]

KAIST 화학과

Developing a new efficient homogeneous catalyst for carbon dioxide (CO_2) conversion is currently receiving great attention due to its relevance to the global energy and environmental issues. In Nature, an efficient catalytic interconversion of CO_2 to CO occurs in carbon monoxide dehydrogenase (CODH) possessing a nickel containing active site. However, initial CO_2 binding to a nickel center is still unclear. Therefore, investigation on the interaction between CO_2 and a nickel center under the similar coordination environment of CODH active site is crucial not only to understand enzymatic conversion of CO_2 but also to develop efficient homogeneous catalysts for CO_2 conversion. Inspired by the active site structure of CODH, a zero-valent nickel center supported by a tridentate ligand, $PP^{Me}P$ ($PP^{Me}P = PMe[2\text{-}P^iPr_2\text{-}C_6H_4]_2$) was prepared by synthesizing a 4-coordinate dinuclear nickel-dinitrogen complex $\{(PP^{Me}P)Ni\}_2(\mu\text{-}N_2)$. A dinitrogen ligand can be easily replaced by CO_2 to generate 5-coordinate nickel-CO_2 adduct $(PP^{Me}P)Ni(\eta^2\text{-}CO_2)$. This is a new type of CO_2 binding mode in a zero-valent nickel center supported by three donor ligands, reminiscent of the CODH active site. Further reactivity of a nickel-CO_2 adduct toward boron containing compounds such as $B(C_6F_5)_3$, HBpin, and B_2Pin_2 was explored. The details of CO_2 conversion at a zero-valent nickel center supported by a tridentate ligand will be presented.



P^iPr_2
P
$Ni(COD)_2$
N_2
C_6H_6
Ni
- N_2
+ N_2
1/2
$N\equiv N$
$^iPr_2P$
+ CO_2
- N_2
C_6H_6
$B(C_6F_5)_3$
C_6H_6
$OB(C_6F_5)_3$
O
C

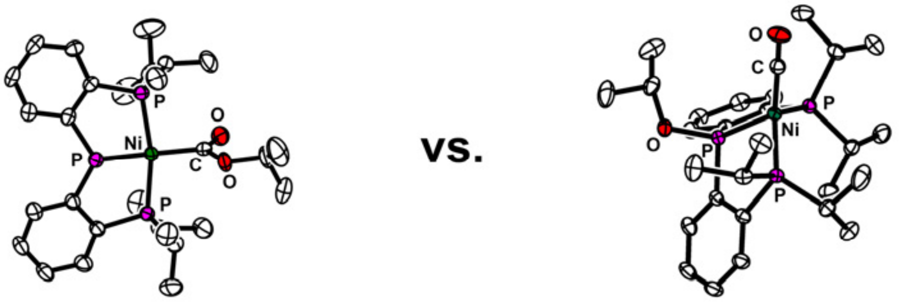
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-160**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal-Ligand Cooperative Isopropoxide Group Transfer from a Single Nickel Center

오서희 이다영 곽진성 이윤호*

KAIST 화학과

Metal-ligand cooperation mediated by non-innocent ligands has received much attention recently as a unique methodology for various transition metal based catalyses. While well-known examples possessing a π-conjugated system as a non-innocent motif such as aryl-substituted bis(imino)pyridine and pyridine/acridine are widely studied, there are relatively few reports in phosphine-based ligands. We recently reported non-innocent activities of an anionic PPP ($PPP^- = P[2\text{-}P^iPr_2\text{-}C_6H_4]_2^-$) ligand with a single nickel ion revealing the reversible transformation between a phosphide-nickel(II) alkoxide and a phosphinite-nickel(0) species via a reversible P-O bond formation/cleavage. In order to further expand this unusual metal-ligand cooperation, we have tried to generate a nickel(II)-alkoxide complex which can be converted to a Ni(0)-phosphinite species in the presence of a π-acidic ligand. With an isopropoxide anion, $(PPP)NiO^iPr$ was synthesized and its reactions with carbon monoxide, isocyanide and carbon dioxide were examined. Upon addition of CO(g), surprisingly a nickel(II) acyl species $(PPP)NiCOO^iPr$ was produced via CO migratory insertion. This result is unexpected when the reaction is compared with previous examples. Analogous phenoxide and phenylthiolate congeners reveal the formation of $(PP^{EPh}P)NiCO$ (E = O, S) from their reactions with CO(g). However, upon addition of CNtBu, P-O bond formation occurs which is coupled with two electron reduction of a nickel center resulted in the formation of a Ni(0) species $(PP^{OiPr}P)NiCN^tBu$. Further details of the reactions will be presented in this poster.Reference[1] Kim, Y. –E.; Oh, S.; Kim, S.; Kim, O.; Kim, J.; Han, S. W. and Lee, Y. J. Am. Chem. Soc. 2015, 137, 4280.[2] Oh, S. and Lee, Y. Organometallics 2016, 35, 1586.



$(PPP)Ni^{II}(COO^{i}Pr)$ **$(PP^{O^{i}Pr}P)Ni^{0}(CO)$**

CO Migratory Insertion **Metal Ligand Cooperation**

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-161**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of 3,4-Diphenyl-1,1-disubstituted-2,5-bis(trimethylsilyl)silole

조윤호 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

1,1-Diisopropyl(and 1,1-Diphenyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)silole were prepared by the intramolecular reductive cyclization of diisopropyl(and diphenyl)bis(phenylethynyl)silane with treatment of 4.5 mol lithium naphthalenide followed by 4 mol chlorotrimethylsilane soluted in THF. After the synthesis, the naphthalene was removed via naphthalene sublimation apparatus, and to increase the yield by recrystallization. The obtained moleculars are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by GPC, NMR, and IR spectroscopies along with TGA. We also studied the electronic properties of the prepared polycarbosilanes by UV-vis absorption, excitation, fluorescence emission spectroscopic methods and cyclic voltammetry, in particular.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-162**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A superior anode material derived from ZIF-8/porous carbon nanocomposites for lithium-ion batteries

김태경 김종식*

동아대학교 화학과

Metal-organic frameworks (MOFs) have been used in many fields such as catalysis, gas storage, and chemical sensing because of their high porosity and large surface area. Recently, MOFs have been further investigated as a precursor of various functional nanomaterials. In this study, ZIF-8, which contains both zinc and nitrogen elements, is embedded in a porous carbon foam through water vapor method. Subsequently, nanosized ZnO-loaded/N-doped carbon composites (ZnO/N-CF) are prepared by the controlled heat-treatment of the impregnated precursors and examined as an anode materials for lithium-ion batteries. Although ZnO suffers from poor cycling stability due to the low electrical conductivity and large volume change during the consecutive insertion–extraction processes of lithium ions, the ZnO/N-CF composites overcame these drawbacks by effectively preventing the aggregation and simultaneously improving the conductivity of the ZnO nanoparticles. The composites exhibited the stable discharge capacities of about 1300 $mAhg^{-1}$ between 0.0-3.0 V at 0.1 C rate. The excellent electrochemical performance is attributed to the synergistic effect of ZnO nanoparticles and conductive N-CF matrix.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-163**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Variable dimensionality and framework in new quaternary zinc selenites

Lu Minfeng 조홍일 오승진 옥강민*

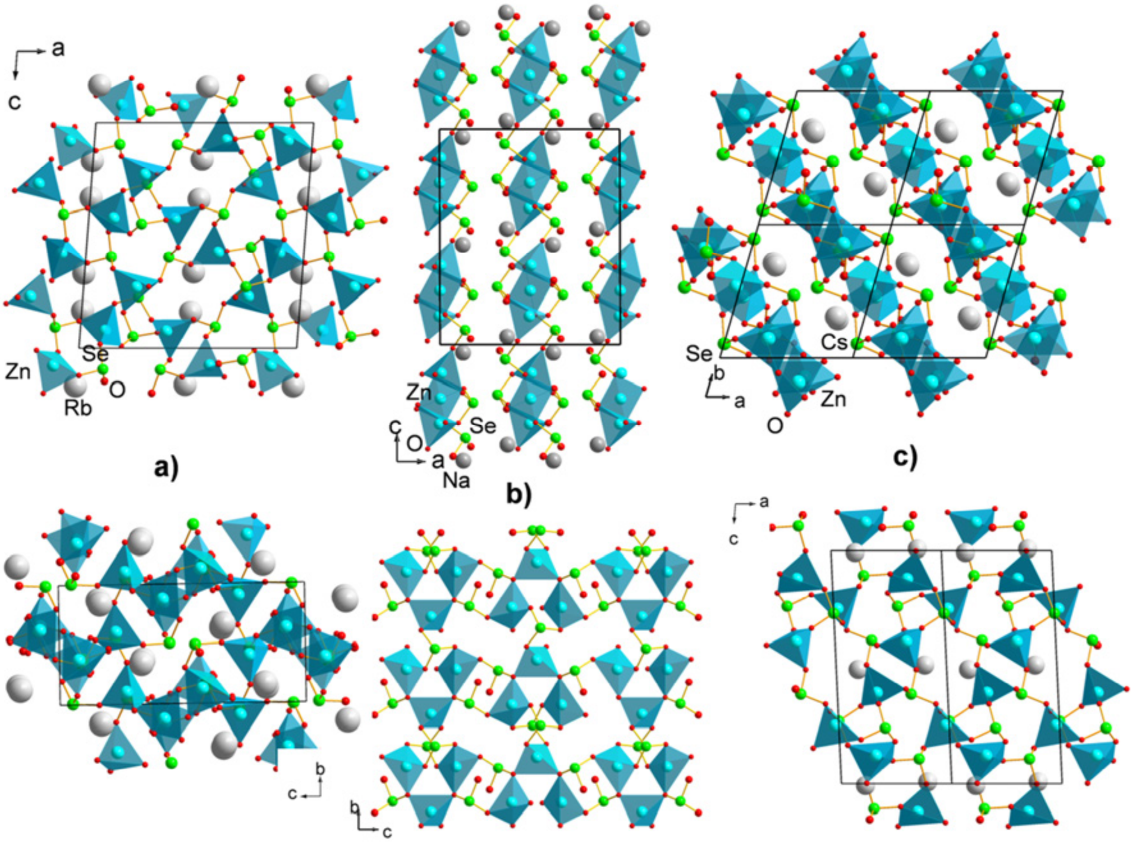
중앙대학교 화학과

The crystal chemistry of selenium(IV) oxides is very interesting since the cation contains a stereochemically active lone pair in the specific trigonal pyramidal geometry, leading to noncentrosymmetric (NCS) structures, and thus their potential applications in nonlinear optical second harmonic generation (SHG)[1, 2]. Moreover, the crystal chemistry of mixed metal selenium oxides revealed abundant structural versatility[3] with a variety of coordination modes such as $HSeO_3^-$,SeO_3^{2-} and $Se_2O_5^{2-}$ oxoanions. With the ulterior motivation of preparing novel transition metal selenites, we synthesized five new alkali metal zinc selenites, $A_2Zn_3(SeO_3)_4 \cdot xH_2O$ (A = Na, Rb, and Cs; $0 \leq x \leq 1$) and $Cs_2Zn_2(SeO_3)_3 \cdot 2H_2O$, which revealed a rich structural chemistry with different frameworks and connection modes of Zn^{2+}. $Rb_2Zn_3(SeO_3)_4$ (Fig.1a) and $Cs_2Zn_3(SeO_3)_4 \cdot H_2O$ revealed three-dimensional frameworks consisting of isolated ZnO_4 tetrahedra and SeO_3 polyhedra, while $Na_2Zn_3(SeO_3)_4$ (Fig.1b), $Cs_2Zn_3(SeO_3)_4$ (Fig.1c), and $Cs_2Zn_2(SeO_3)_3 \cdot 2H_2O$ contained two-dimensional $[Zn_3(SeO_3)_4]^{2-}$ layers. Specifically, whereas isolated ZnO_4 tetrahedra and SeO_3 polyhedra are arranged into two-dimensional $[Zn_3(SeO_3)_4]^{2-}$ layers in two cesium compounds, circular $[Zn_3O_{10}]^{14-}$ chains and SeO_3 linkers are formed in two-dimensional $[Zn_3(SeO_3)_4]^{2-}$ layers in $Na_2Zn_3(SeO_3)_4$.

1. K. M. Ok, P. S. Halasyamani, Chem. Mater., 2002, 14, 2360.

2. S.-J. Oh, D. W. Lee, K. M. Ok, Inorg. Chem., 2012, 51, 5393.

3. A. Larranaga, J. L. Mesa, J. L. Pizarro, R. Olazcuaga,. M. I. Arriortua, T. Rojo, Dalton Trans., 2002, 3447.


a
c
Se
Zn
O
Rb
a)
Zn
Se
c
O
a
Na
b)
Se
b
a
Cs
Zn
O
c)
b
c
b
c
a
c

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-164**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Patterned Growth and 2D Structure of Covalent Organic Frameworks (COFs) via Ultrafast Photochemical Synthesis

김소영 최희철*

POSTECH 화학과, 기초과학연구원 CALDES

Covalent organic frameworks (COFs) are crystalline organic building block, which are linked by covalent bond between light elements. Since the first report on COFs in 2005 they have been widely studied as potential next-generation materials for gas storage and chemical catalysts because of their high thermal stability and stable porosity. In addition, they were further expected as superior two-dimensional nanomaterials which shows remarkable charge transfer and separation properties across π-conjugated layers. In spite of these advantages of COFs, however, the current solvothermal synthesis procedure has limitations such as long synthesis time (2~7 days) and high reaction temperature (90~120 °C).Herein, we have successfully synthesized COF-5 having highest surface area among previously reported by using light irradiation. Light-induced method significantly reduces reaction time down to a few hours at room temperature, which is dramatically milder condition than that of conventional solvothermal method (3 days, 90 °C). Moreover, by using the strength of light, we have succeeded in patterning the COF-5 into various geometry on a SiO_2 substrate at the desired positions, exploiting the unique advantages of light as the energy source. Also, as an application perspective, a few atomic layer COF was synthesized by light irradiation and solvent instability. From this result, it was proved light irradiation can be a good energy source in COF synthesis and application, especially in device fabrication for diverse application like gas sensing, catalyst and etc.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-165**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Synthesis and Electrical Characterization of Alkali metal doped Picene Single Crystal

이진호 최희철*

POSTECH 화학과, 기초과학연구원 CALDES

After the discovery of the superconductivity from alkali-doped hydrocarbons, highly conjugated molecules have gained great interests as a new family of superconducting materials. Especially among these molecules, alkali-doped picene shows multiple superconducting phases, which has different T_c with same stoichiometric composition. A possible explanation to this phenomenon suggests that the different position of dopants within the crystal lattice may be related to the different T_c. Therefore, the control of the T_c in hydrocarbon-based superconducting materials require a more in-depth study of the correlation between the crystal structure and the superconductivity. In this respect, organic single crystal in which the crystal lattice of the sample is continuous with no grain boundaries is more suitable specimen to research rather than powder or polycrystalline samples. In this presentation, we report that the single crystals of picene have been doped by potassium with our homemade doping system, and the doped phase of picene shows the enhancement of the conductivity. We prepared the picene single crystals by drop drying method and made the doped phase in dynamic vacuum system. We confirmed the uniformly doped picene crystal with raman spectrum. With X-ray diffractions, we could find that dopants could exist between ab plane, which is different results from the previous report. By measuring the transport experiment, we could observe dramatic change in conductivity after the doping process.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-166**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solid Substrate-Dependent Control of Growth Direction of *p*-terphenyl Crystals

박지원 최희철*

POSTECH 화학과, 기초과학연구원 CALDES

The rational design of exposed crystal facets allowed the development of organic crystal without changing material compositions. Each crystal facet would have different optical, electrical, or magnetic properties, and control of each phase considered important factor for the nanoscale device application. However, because crystal growth mechanisms are not fully understood, control of crystal morphology/facet still remains unexplored. Herein, we applied solid substrate-dependent crystallization technique using physical vapor transport (PVT) method to control the exposed crystal facet. We used graphene as two-dimensional material and *p*-terphenyl as the organic molecule to control growth direction so as to do changing crystal packing, and to study improved characteristics of the *p*-terphenyl. Interestingly, we found the different crystal growth patterns depending on substrates (graphene/SiO_2). *p*-terphenyl crystals with vertical and disk morphology were grown on the graphene substrate, whereas lateral crystal, which has not specific morphology were grown on the SiO_2 substrate. To analyze crystal structure, we conducted powder X-ray diffraction (PXRD) and it indicates crystalline structures. In addition, we carried out photoluminescence (PL) of the *p*-terphenyl on each substrate and it shows increased properties on the graphene substrate.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-167**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Sudden magnetic properties changing in alkali metal doped triphenylene

윤태경 최희철*

POSTECH 화학과, 기초과학연구원 CALDES

After first discovery of superconductivity in only carbon based graphite intercalation compounds (GICs) in 1965, light-element superconductors (LEMs) consisted of light atoms such as boron, carbon, nitrogen have been received huge amount of attraction. In spite of their low critical temperature in comparison to inorganic superconductors, they have been studied intensively because they have lots of advantages like low toxicity, abundant quantity, cheaper price and lighter weight.One of the core category of LEMs is hydrocarbon molecules only formed with carbon and hydrogen. In particular, polycyclic aromatic hydrocarbons (PAHs) made up of sp2 carbons and fused benzene-ring structures have taken significant interest because of their extended pi-bonds and delocalized electrons which are regarded as a key role of organic superconductors. Due to their lack of charge carrier density, they needs additional electrons by injecting alkali(-earth) metal, and it make it difficult to develop various PAH superconductors.Thus in this work, we are going to report new PAH superconductor candidate ‘Alkali metal doped triphenylene’. They were synthesized in vacuum sealed glass tube to prevent contact with oxygen and annealed at adequate temperature. In case of superconducting samples, they show sudden drop of magnetic susceptibility which means Meissner effect below 14 kelvin.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-168**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Organic Heterostructure Formed by Molecular Conversion of Anthracene Single Crystal

이민경 최희철*

POSTECH 화학과, 기초과학연구원 CALDES

The organic materials have been widely studied for optoelectronic device applications such as organic display, laser, and organic field effect transistors. Recently, controlling organic heterostructure is gathering great attention since it is one of the most important factor for modulation of the electrical and optical properties. So, many researches have studied organic / organic heterostructure in thin film or well-defined crystal with phase separation or ordered complex effect. Here, we present anthraquinone disk was synthetized from anthracene disks through photooxidation (or photodimerization) of anthracene molecules in ambient (or argon) condition. Upon ultraviolet (> 300 nm) light illumination in the presence (absence) of oxygen, the anthracene with monoclinic structure rearrange to the anthraquione (dipara-anthracene) disk with monoclinic (orthorhombic) structure. The photoluminescence property shows definite difference between anthracene, anthraquinone and dipara-anthracene disk. In case of anthraquinone disk is also different with that of anthraquionoe powder. The anthraquinone disk presents red photoluminescence which is attributed to the remained anthracene. In addition, organic/organic heterostructure fabricated by using shadow mask.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-169**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular Level Chromophore-Catalyst Assemblies for Dye-Sensitized Photoelectrosynthesis Cells (DSPEC)

위경량

대구대학교 화학응용화학과

We describe stability and efficiency of donor-p-acceptor (D-p-A) organic dye (OrgD-P) based molecular level chromophore-catalyst assemblies in aq. solution for water oxidation dye-sensitized photoelectrochemical cell (DSPEC). As shown by electrochemical stability in aq. pH 1, the stability of radical cation species of OrgD-P exhibits scan rate dependent properties showing almost no decomposition at higher scan rate of >400 mV/s. Also in the photostability experiment, we observed the full loaded OrgD-P on the mesoporous TiO2 film is photochemically stable and reduces desorption of OrgD-P from the surface during the light irradiation in aq. solution while the partially loaded film was unstable due to its self-protecting of the anchoring group by hydrophobic linear-shape D-p units. In the photocurrent measurement, FTO|TiO2-OrgD-P shows less than 5 microA in pH 7 phosphate buffer solutions under light illumination (100mWcm-2) but ~100-fold enhanced photocurrent in the core-shell electrode of FTO|SnO2@TiO2-OrgD-P due to the dramatically reduced back electron transfer process of OrgD-P on the core-shell nanoparticle. In particular, FTO|SnO2@TiO2-OrgD-P film shows high photocurrent density of >2.6 mA without reduced current for the 15 min in the present of 20 mM of hydroquinone (H2Q) as an external donor. Finally, molecular assembly of OrgD-P and water oxidation catalyst by co-loading method on the SnO2@TiO2 films provides the basis for a DSPEC for water splitting and photoinduced oxygen generation was measured in real-time by use of a two-electrode cell.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-170**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Progress toward N-Heterocyclic Carbene Based MOFs Using Pyrazolyl Imidazolium Ligands

이재철 노경규[1] 김자헌[1] 김기문 이은성*

POSTECH 화학과 [1]숭실대학교 화학과

Metal–organic frameworks (MOFs) have attracted great interest due to their potential applications such as catalysis, gas storage, and separation of molecules. Organic linkers bearing N-heterocyclic carbenes (NHCs) have been emerging for supporting various transition metals catalysts in MOFs. However, there is a little study on intrinsic properties of free NHC in MOFs although N-heterocyclic carbenes (NHCs) are well-known to activate small molecules such as CO_2, CO, NH_3 and H_2 or even to stabilize main group radicals.[1] One of the major problems in synthesizing NHC MOFs from carboxylated imidazolium ligands was found that the frameworks were collapsed upon the deprotonation of the imidazolium ligands with strong bases to access free NHCs. Since pyrazolate-based MOFs are well known to have a good stability under basic conditions, we synthesized a couple of pyrazolyl imidazolium ligands and succeed to make new imidazolium MOFs from the ligands. The properties of the MOFs and progress to access pyrazolyl imidazolium MOFs will be presented.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-171**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Tungsten Diselenide film *via* Metal-Organic Chemical Vapor Deposition

이유빈 정희경 박이슬 이진석*

숙명여자대학교 화학과

Beyond graphene, transition metal dichalcogenides (TMDC) are interested owing to their optical, electronic properties. Synthesis of monolayer of tungsten diselenide (WSe_2) by chemical vapor deposition (CVD) method has researched variously. But, one of the spotlighted synthesis techniques, metal organic chemical vapor deposition (MOCVD) for synthesis TMDC materials has not been actively reported yet.Here, we present the report of synthesis WSe_2 films *via* metal organic chemical vapor deposition method using tungsten hexacarbonyl ($W(CO)_6$) and dimethyl selenide ($Se(CH_4)_2$) on silicon oxide substrate [1] and characterized by atomic force microscopy (AFM). We controlled their film height by changing the ratio of carrier gas and pressure, which resulted in mono- and few-layer of produced WSe_2 film. Also we observed E^{1}_{2g} and A_{1g} mode, two main Raman modes of WSe_2, using micro-Raman spectroscopy that they are detected different intensity respectively [2], [3].Reference[1] Eichfeld, S.; Hossain, L.; Lin, Y.; Piasecki, A.; Kupp, B.; Birdwell, A.; Burke, R.; Lu. N.; Peng, X.; Li, J.; Azcatl, A.; McDonnell, S.; Wallace, R.; Kim, M.; Mayer, T.; Redwing, J.; Robinson, J. ACS Nano. 2015, 9, 2, 2080-2087.[2] Lee, C.; Yan, H.; Brus, L.; Heinz, T.; Hone, J.; Ryu, S. ACS Nano. 2010, 4, 5, 2695-2010.[3] Chen, S.; Zheng, C.; Fuhrer, M.; Yan, J. Nano Letters. 2015, 15, 2526-2532.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-172**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Single Atom and Molecule Manipulation and Spectroscopy on Noble Substrate with a Scanning Tunneling Microscope

권태연 최희철[*]

POSTECH 화학과, 기초과학연구원 CALDES

Organic and inorganic molecular nanostructures are analyzed by various spectroscopic method. Recently, atomic level measurement is gathering great attention because it provide opportunities for fundamental researches, also new properties development. So, many researcher have been studied molecule characterization or chemical reaction by using scanning tunneling microscope (STM). Here, we present that lanthanide atoms (dysprosium and holmium) and fluorinated copper phthalocyanine (Copper(II) 1,2,3,4,8,9,10,11,15,16,17,18,22,23,24,25-hexadecafluoro-29H,31H-phthalocyanine; F_{16}CuPc) were manipulated by silver tip on noble metal substrate, and measured electronic properties by homemade various temperature STM. We found that a triangle shaped nanocomplex which is made by lateral manipulation in STM has a weak interaction. Furthermore, we have been interested in magnetic properties of molecular structures. For magnetic properties measurement, sub Kelvin and 7 Tesla cryostats is under constructing. We hope nanostructures made by manipulation can change spin state, and this spin controlling between magnetic atom and molecules can be contributed to spintronic or single molecular magnets (SMM).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-173**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Hybrid Organic-Inorganic Alucone Film Growth Using Molecular Layer Deposition

김혜인 최의진 박이슬 이진석*

숙명여자대학교 화학과

Molecular layer deposition (MLD) is a method for obtaining conformal ultrathin organic films using vapor-phase organic precursors, while their composition and thickness can be controlled at the molecular level. This process is based on self-saturating reactions between the organic precursors and the substrate surface. Also, in comparison with solution-based technique, it allows epitaxial growth of molecular layer on substrate and is especially good for surface reaction or coating of nanostructures such as nanopore, nanochannel, nanowire array and so on.In this study, we fabricated organic-inorganic alucone polymeric films through coupling reactions between trimethyl aluminum (TMA) and one of two diols with different carbon-carbon bond order as inorganic and organic precursors, respectively, by molecular layer deposition. Using ellipsometry, we confirmed linear growth of the films versus number of MLD cycles at all same temperature. The mass gains in alucone films grown with varying doses of TMA and organic diol were identified using in situ quartz crystal microbalance (QCM) technique. This presents different tendency of the mass gain of the films to reduce with increasing of the flexibility of organic precursors. And, surface potential of alucone films were investigated by ex situ analysis scanning kelvin probe microscopy (SKPM). Furthermore, all molecular geometries and doubling energies were predicted by performing density functional theory (DFT) calculations.Reference[1] J. S. Lee; Y. -J. Lee; E. L. Tae; Y. S. Park; K. B. Yoon, Science, 2003, 301, 818−821.[2] A. A. Dameron; D. Seghete; B. B. Burton; S. D. Davidson; A. S. Cavanagh; J. A. Bertrand; S. M. George, Chem. Mater. 2008, 20, 3315–3326.[3] A. I. Abdulagatov; R. A. Hall; J. L. Sutherland; B. H. Lee; A. S. Cavanagh; S. M. George, Chem. Mater. 2012, 24, 2854−2863.[4] Y.-S. Park, S.-E. Choi, H. Kim, J. S. Lee*, ACS Applied Materials & Interfaces, 2016, 8 (18), 11788–11795.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-174**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anionic metal-organic framework containing one-dimensional channels

우경택 최예진 김자헌*

숭실대학교 화학과

A solvothermal reaction between 2-fluoro-1,3,5-benzene-tricarboxylic acid (BTC-F) and with Zn(II) resulted in a three-dimensional metal-organic framework (Zn-BTC-F-1) having straight channels with hexagonal openings. The crystal structure revealed that the framework has negative electric charges compensated with octahedral $[Zn(DMF)_3(OH_2)_3]^{2+}$ complexes present in the channels of Zn-BTC-F-1. Part of the cationic guest complexes could be replaced with external metal ion, Tb(III), which made the host crystal emit luminescence when excited at 350 nm. The preparation, crystal structure of Zn-BTC-F-1, and its cation exchange experiments as well will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-175**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Control of the Water Adsorption Properties of Metal-Organic Frameworks by Linker Functionalization

윤하경 오유진 김자헌*

숭실대학교 화학과

Two pristine metal-organic frameworks (MOFs), Al-MIL-160 and Cr-MIL-101 were respectively modified in order to make them adsorb water vapor in a desired pressure range, $P / P_0 = 0.1 \sim 0.3$. In the case of Al-MIL-160, a direct synthesis was applied to make a series of mixed-ligand MOFs. In contrast, a step-by-step chemical modification of the framework linkers in Cr-MIL-101 was employed for making the pore surfaces more hydrophilic. Water adsorption measurements indicated that the functionalized Al-MIL-160 showed an S-shaped water uptake at $P/P_0 = 0.25$ whereas the modified Cr-MIL-101 adsorbed water vapor at $P/P_0 = 0.35$.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-176**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Syntheses of functionalized ZIF-8 compounds via successive ligand insertion to a metastable zeolitic-imidazolate framework

최예진 우경택 김자헌*

숭실대학교 화학과

ZIF-8 is a sodalite-like zeolitic-imidazolate framework (sod ZIF) with Zn(mIm)$_2$ (mIm = 2-methylimidazolate) as a formula. Unlike known procedures, ZIF-8 with mixed imidazolates could be prepared from a metastable ZIF exhibiting pcb topology (pcb ZIF). First, mIm was partially inserted into pcb ZIF, accompanied by a structure transformation to a sod ZIF formulated as Zn(Im)$_{1-x}$(mIm)$_x$ (ZIF-8x). Then, various imidazolates with different functional groups could be further inserted into ZIF-8x to produce a series of MTV-ZIF-8 compounds: MTV = multi-variate. The unique and interesting gas adsorption properties of the MTV-ZIF-8s are to be presented.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-177**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Scale-up synthesis of water-stable Al-fumarate

남지은 노경규 김자헌*

숭실대학교 화학과

Al-fumarate is formulated as Al(OH)(fumarate), and has a similar structure with that of Al-MIL-53. Al-fumarate is very stable in water, and shows steep and large water uptake of 0.30 g/g at $P/P_0 = 0.25$. Due to this novel property, Al-fumarate is considered as one of the most promising water sorbents. Since an easy and inexpensive preparation method of Al-fumarate is required for practical applications, we have developed a simple precipitate method in water at ambient temperature. In this presentation, we will show the optimized scale-up procedure, and compare the water adsorption properties of several Al-fumarate products obtained respectively with different preparation methods. The result on the water adsorption-desorption cycling test for Al-fumarate will be also presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-178**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Four metal-organic frameworks from nitro-functionalized biphenyl-dicarboxylic acid and Cu, Co, or La ion

노경규 심재웅[1] 김자현*

숭실대학교 화학과 [1]UNIST 자연과학부

2,2',6,6'-Tetranitro-biphenyl-4,4'-dicarboxylic acid was employed to make nitro-functionalized metal-organic frameworks (MOFs); a **cds** Cu-MOF, an **nbo** Cu-MOF, a **bcu** Co-MOF, and a **bct** La-MOF were obtained respectively with Cu, Co, and La ion through solvothermal reactions. Due to the nitro functional groups densely decorating organic linkers, all the MOF crystals were explosively decomposed around 250℃ based on TGA measurements. Among the MOFs, the porosity and gas adsorption properties of the **cds** Cu-MOF were investigated in detail, and the results will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-179**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Zn_2SnO_4/N-doped Carbon Using Dopamine as an Anode Material for Lithium-Ion Batteries

김남영 김종식*

동아대학교 화학과

Lithium-ion batteries (LIBs) have been commonly used in electric devices including convenient electronic applications and electric vehicles because of these advantages such as lightweight, high power density, and high energy density. However, the current LIBs are still required to improve the rate capability, short cycle life, cycling stability, and discharge capacity. Zinc stannate (Zn_2SnO_4) is one of the attractive anode materials for LIBs due to its easy preparation, high electrical conductivity, low cost, and high specific capacity of about 1231mAhg-1. Despite these merits, Zn_2SnO_4 often shows poor cycling stabilities because the large volume changes and particle pulverization occur during Li-insertion/extractions on repeated cycling. In this work, N-doped carbon-coated Zn_2SnO_4 (Zn_2SnO_4/NC) composites were synthesized via a facile hydrothermal method using dopamine, which contains catechol and amine groups and thoroughly characterized by XRD, SEM, FT-IR. The Zn_2SnO_4/NC shows the enhanced electrochemical performance compared to bare Zn_2SnO_4 at current density of 60 mA/g in the voltage range of 0.005-3.0 V.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-180**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Palladium(II) complexes containing acac(α-acetylacetone) and NHC ligands with bulky aryl group and their catalytic activity towards norbornene polymerization

이동진 이익모*

인하대학교 화학과

Pd(II) complexes containing various NHC(N-heterocyclic carbene) ligands have been successfully synthesized by the reaction with acac(α-acetylacetone).Treatments of Pd(α-acac)2 with NHC salt such as IPr·HCl, IMes·HCl resulted in [Pd(α-acac)(NHC)Cl] complexes and these complexes are characterized by NMR and elemental anaylsis.Moreover, these new palladium complexes showed moderate to good catalytic activities towards norbornene polymerization.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-181**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photo-activated NO-releasing Ruthenium Nitrosyl Complexes

김민영 이홍인* 조장훈 임만호[1]

경북대학교 화학과 [1]부산대학교 화학과

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, nitrosyl ruthenium complexes have been proposed as attractive photodynamic therapeutic agents in biomedicine and in tumor treatment. This research aims at developing nitrosyl ruthenium complexes which absorb long wavelength visible light to release NO with high quantum yield. Previously, we have developed a new Ru-nitrosyl bis-pyridyl/biscarboxamide compound, [Ru(III)(ebpp)(Cl)(NO)], where H2ebpp = N,N'-(ethylene di-p-phenylene)bis(pyridine-2-carboxamide), to be tested as a model NO-releasing agent. Here, we present the strategies to develop visible-light sensitive NO-releasing Ru complexes with higher quantum yield. We introduced new series of ligands, bis-salophen and bis-naphophen, to develop Ru-nitrosyl complexes. In this study, we describe our progress in designing photoactive ruthenium nitrosyls and the properties of the photo-activated NO-releasing of the complexes monitored by UV-VIS, EPR, X-ray crystallography and femtosecond mid-IR spectroscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-182**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tripodal shaped ligand for catalyst for copolymerization of CO2 and epoxide

임영재 허정석*

충남대학교 화학과

For last few decades, carbon dioxide has been considered one of the main cause leading to the green house effect. To reduce the amount of the gas, many applications on the issue have been performed and CO2 and epoxide copolymerization has been regarded as a promising approach which can use CO2 as one of resources. We prepared a ligand as a catalyst precursor by coupling 1,1-tris(3-formyl-4-hydroxyphenyl)ethane and 2-amino-4-chlorophenol the catalyst precursor was successfully characterized by 1H-NMR spectroscopy and single-crystal X-ray diffraction crystallography. Interestingly in X-ray crystal, the tripodal ligands assembled via multiple hydrogen bondings to form tetrameric cluster. Details of this work will be presented in the poster presentation

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-183**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Host-Guest Interactions of Homochiral Molecular Baskets

임영재 허정석*

충남대학교 화학과

Homochiral supramolecular assemblies are of great interest owing to their potential applications in chiral separations, sensing and enantioselective synthesis of important bioactive chemicals. We prepared a basket shape of macrocyclic compound by coupling (1,1’-biphenyl)-3,5-dicarboxaldehyde and (1S,2S)-(+)-1,2-cyclohecanediamine as a host molecule for chiral compounds like mandelic acid and mandelonitrile. We also reduced the imine type of cage molecule to stabler amine type of cage and studied host-guest interactions with both cage and chiral guest molecules by monitoring 1H-NMR chemical shifts. Detailed synthetic procedures of molecular baskets, characterizations, and binding study results will be presented in the poster session.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-184**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Four-coordinate nickel nitrosyl complexes supported by a tridentate pincer type PEP ligand

곽진성 이윤호*

KAIST 화학과

The reactivity of transition metal nitrosyl complexes is of particular interest in our research. This is due in part to the fundamental understanding of metal nitric oxide (NO) species relevant to the extensive roles of nitric oxide (NO) in biology, which involves an integral part of immune response, vasodilatation, and neurotransmission. Recent researches revealed that reactive nitrogen species (RNS) might be generated from the interaction of NO with various reactive oxygen species (ROS) mediated by transition metal ions in biological systems. Our current investigation focuses on the chemistry of metal nitrosyl species in particular with a nickel ion. To date, structurally characterized nickel nitrosyl complexes reported in literature feature only an Enemark-Feltham configuration of $\{Ni(NO)\}^{10}$. Despite this lack of diversity, recent works revealed that nickel nitrosyl complexes can exhibit a diverse range of reactivity such as dissociation, disproportionation, and reduction.Recently, we have synthesized dinuclear nickel dinitrogen complexes $\{(PP^RP)Ni\}_2(\mu\text{-}N_2)$ with tridentate PP^RP ligands; $PP^RP = P(R)(2\text{-}P^iPr_2\text{-}C_6H_4)_2$, (R = Ph and Me). A series of tetrahedral nickel nitrosyl complexes $[(PP^RP)Ni(NO)][BF_4]$ were prepared by the reaction of dinuclear nickel dinitrogen complexes with nitrosonium ion ($NOBF_4$). According to spectroscopic and structural data, these nickel complexes possess a $\{NiNO\}^{10}$ moiety. In fact, a neutral paramagnetic nickel nitrosyl species $(PP^RP)Ni(NO)$ featuring an unusual $\{Ni(NO)\}^{11}$ configuration was prepared by the chemical reduction of $[(PP^RP)Ni(NO)][BF_4]$. As a closely analogous square planar nickel nitrosyl complex (PNP)Ni(NO) with a tridentate PNP– ligand; ($PNP^- = N[2\text{-}P^iPr_2\text{-}4\text{-}Me\text{-}C_6H_3]^{2-}$) was also prepared by oxygen atom transfer reaction. Distinct difference can be recognized in its metal nitrosyl moiety, NiI-NO• by comparing with the PPP analogue. In order to highlight their electronic features, details of nickel nitrosyl species will be presented including their characterizations with various spectroscopic techniques.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-185**

발표분야: 무기화학

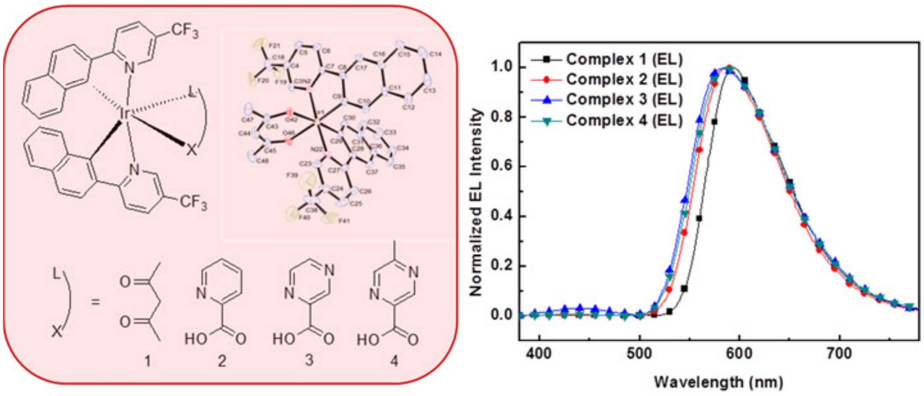
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel Orange-Red Phosphorescent Iridium(III) Complexes Containing 2-(Naphthalen-2-yl)-5-(trifluoromethyl)pyridine for Organic Light-Emitting Diodes (OLEDs)

윤성재 전진실[1] 전종호[2] 김영인[1,*]

한국원자력연구원 생명공학연구부 [1]부산대학교 화학교육과 [2]한국원자력연구원 첨단방사선 연구소

Normally, the emission wavelength of an Ir(III)-phenylpyridine (ppy) complex is red-shifted when an electron-withdrawing group is added to the pyridyl moiety of ppy or an electron donating group is introduced to the phenyl moiety of ppy, the π-conjugation length of the ligand is extended. In this study, the electron-withdrawing trifluoromethyl group in the pyridyl moiety and aromatic group in the phenyl moiety of ppy ligand were introduced to tune the energy band gap of the complexes. The efficient cyclometalated iridium(III) complexes with variety ancillary ligands were synthesized and characterized ; (nptfpy)$_2$Ir(acac) (1), (nptfpy)$_2$Ir(pic) (2), (nptfpy)$_2$Ir(prz) (3) and (nptfpy)$_2$Ir(mprz) (4) (nptfpy = 2-(naphthalene-2-yl)-5-(trifluoromethyl) pyridine ; acac = acetylacetone ; pic = picolinic acid ; prz = pyrazine-2-carboxylic acid and mprz = 5-methylpyrazine-2-carboxylic acid). The complexes exhibited the photoluminescence at 572 ~ 587 nm in solution. The solution-processed OLEDs with the configuration ITO / PEDOT:PSS / TPD:PBD:Ir(III) complexes / TPBi / LiF / Al were performed and the best performance on compound 1 showed an external quantum efficiency of 10.4 %, luminance efficiency of 21.0 cd/A and power efficiency of 9.4 lm/W. The iridium(III) center of complex 1 adopts a distorted octahedral coordination geometry with cis metalated carbon and trans nitrogen atoms and there is a π-π interaction between two naphthalene ring of nptfpy ligand.


CF3
N
Ir
L
X
N
CF3
L
X
=
O
O
1
N
HO
O
2
N
N
HO
O
3
N
N
HO
O
4
Complex 1 (EL)
Complex 2 (EL)
Complex 3 (EL)
Complex 4 (EL)
Normalized EL Intensity
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
400
500
600
700

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-186**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on crystal structures and properties of trinuclear nickel(II) and cobalt(II/III) complexes with tetradentate N_2O_2-type ligands

정아림 민길식[1,*]

경북대학교 화학과 [1]경북대학교 사범대학 화학교육과

N-(2-pyridylmethyl)iminodiethanol (H_2pmide) and *N*-(2-pyridylmethyl)iminodiisopropanol (H_2pmidip) ligands having a pyridine, an amine, and a hydroxyl group are considered to have the potential to form multinuclear coordination compounds with transition metal ions. Recently, three novel trinuclear complexes, $[(Hpmide)_2Ni_3(OAc)_4]$ (**1**), $[(Hpmide)_2Co_3(OAc)_4]$ (**2**), and $[(pmidip)_2Co_3(OAc)_4]$ (**3**), have been prepared by the N_2O_2-type ligands, H_2pmide and H_2pmidip, with nickel(II) and cobalt(II/III) ions. Complexes **1** and **2** are isomorphous. In **1** and **2**, two terminal nickel(II)/cobalt(II) units are coordinated $Hpmide^-$ and two acetate anions, respectively. The central nickel(II)/cobalt(II) ion is bonded to four oxygen atoms of acetate anion and to two bridged oxygen atoms of Hpmide ligand, respectively. In **3**, two terminal cobalt(III) ions are coordinated to pmidip- and two acetate anions. The terminal units are each linked to a central cobalt(II) cation through two oxygen atoms of $pmidip^-$ and one oxygen atom of acetate anion, giving rise to a linear trinuclear mixed-valence cobalt complex. Complex **1** and **2** shows a weak ferromagnetic and antiferromagnetic interaction through the bridging oxygen atoms, respectively. Additionally, complex **3** behaves as a paramagnetic cobalt(II) monomer, due to the diamagnetic cobalt(III) ions in the terminal units. Unfortunately, there is no catalytic activity in complex **1**. However, **2** and **3** showed significant catalytic activities toward various olefins with modest to good yield. In this poster, we will present the detailed preparation of the ligand and cobalt compounds, crystal structures, magnetic and catalytic properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-187**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel Aluminum-Triarylborane (TAB) Dyads: Synthesis and Their Intriguing Optical Properties via Photoinduced Energy Transfer

곽상우* 최병훈[1] 이강문[1] 정용석 박명환[2,*]

충북대학교 화학과 [1]강원대학교 화학과 [2]충북대학교 화학교육과

The aluminum salen complexes have widely been investigated as outstanding luminophores in diverse optoelectronic materials due to their prominent photophysical properties. Along with these studies, several heterodinuclear systems based on Al-salen complexes have recently been reported. In particular, Al-BODIPY dyad systems exhibited intriguing luminescent properties such as dual emission features via photoinduced energy transfer. In this regard, we chose triarylborane (TAB) moieties as another group connecting to aluminum salen complexes. The TAB compounds have also received a great deal of attention as promising anion sensors. This features originated from electron deficient characters of tri-coordinate boron center. In a continuous effort to develop a novel class of Al-based dyad systems, we newly designed Al-TAB dyad systems. The detailed synthesis, characterization, and optical properties of the dyads with theoretical calculations will be described.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-188**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Optical Properties of Aluminum-o-Carborane Dyads

이선희 곽상우[1] 최병훈[2] 이강문[2] 박명환*

충북대학교 화학교육과 [1]충북대학교 화학과 [2]강원대학교 화학과

The aluminum-based dyad systems such as Al-salen/Ir and Al-salen/BODIPY have been recently reported as prominent luminophores due to their unique optical properties. These features resulted from the efficient energy transfer between the two moieties. On the other hand, to date, a number of o-carborane (o-CB) derivatives have been reported. The o-carborane-based compounds showed intriguing optical properties originating from their intirinsic characters such as electron-withdrawing effects. In this regard, we newly designed Al-o-carborane dyad systems as a novel class of luminophore. The detailed synthesis, characterization, and photophysical properties of the dyads will be described.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-189**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anisotropic Growth of Tungsten Diselenide Domains *via* Chemical Vapor Deposition

정희경 이유빈 이진석*

숙명여자대학교 화학과

Recently, atomically thin Transition Metal Dichalcogenides (TMDC) have attracted much attention, because of their interesting electronic, optical, mechanical properties, and ambipolar transport behavior. Among large numbers of TMDC, monolayer of tungsten diselenide (WSe_2) is of particular interest since it possesses a direct band gap. Recently, Chemical Vapor Deposition (CVD) method has been one of the important and reliable techniques for the synthesis of 2D-material.In this presentation, we will discuss various WSe_2 domains with anisotropic shapes grown on sapphire substrate (c-plane, (0001)) via CVD using tungsten oxide (WO_3) and selenium (Se) powder such as precursors. Generally, the shape of produced WSe_2 domain is known to triangle, but we controlled its shape by changing the amount and position of Se powder, which have cross, tetragon, and circle shapes. Furthermore, we characterized their edge structures by strain-induced Raman spectroscopy using linearly polarized light, and proposed the mechanism for anisotropic domain growth depending on the amount of supplied Se precursor.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-190**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Preparation of Hybrid Metal-Organic Frameworks of $\{Fe_xM_yM'_{1-x-y}\}$-MIL-88B and Use of Anions to Control Their Structural Features

지호연 최소라 오문현*

연세대학교 화학과

The hybrid MOFs, which contain the mixed metal ions or the mixed organic linkers rather than a single kind of metal ion or organic linker, are considered as the quite interesting materials, since they can show the enhanced or irregular properties. In addition to the components, the structural features of MOFs are critical in defining their properties and thus their applications. Herein, we report the preparation of well-controlled hexagonal rod-shaped micro-MOFs of $\{Fe_xM_yM'_{1-x-y}\}$-MIL-88B (M and M′ = Ga, Co, or Mn) containing two or three kinds of metal ions. The effect of the anion on the structural features of MIL-88B was clearly proved by constructing the MIL-88B structures with closed, semi-open, and open forms using acetylacetonate, nitrate, and chloride anions, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-191**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Preparation of Au or Ag Nanoparticles-Embedded Hollow Carbon Spheres from Metal-Organic Frameworks and Their Catalytic Activities

김두영 최소라 오문현*

연세대학교 화학과

Noble metal nanoparticles have received much attention because of their many useful applications such as in catalysis, gas sensing, and energy conversion. However, they are easily agglomerated during the reactions due to their high surface energy; thus, their activity after a reaction is typically less than the initial activity. In current, many efforts have been dedicated to the construction of hybrid composites to prevent the agglomeration of nanoparticles and to retain their activity. Herein, we report a simple approach for the production of Au or Ag nanoparticles-embedded hollow carbon spheres (M@HCS, M = Au or Ag) by one-step pyrolysis of core-shell type MOF hybrids, consisting of polystyrene core and MOF shell loaded with Au or Ag metal ions. As a result of their unique structure, the resulting M@HCS displayed an efficient catalytic activity and also showed an excellent recyclability.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-192**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Hydrogenation of CO_2 Catalyzed by PNP Cobalt Complexes

최종훈 이윤호*

KAIST 화학과

The atmospheric concentration of CO_2 has been increased to an unprecedented level due to a higher rate of fossil fuel combustion. Conversion of CO_2 to the useful chemical products is one of the solutions for such global problem. However, this task is fairly challenging because of the thermodynamically stable character of CO_2. To overcome such limit, harsh conditions including high temperature, high pressure and strong nucleophiles are needed although homogeneous transition metal complexes are added as a reaction catalyst. Development of efficient catalysts is obviously desirable with its proper economical merit. As our particular research interest, the hydrogenation of CO_2 catalyzed by 1st-row transition metal is currently under investigations. Although significant advances were recently achieved with precious and rare-earth metals such as iridium, rhodium and ruthenium, limited catalytic systems based on earth abundant 1st-row late transition metal complexes were reported. The proper catalyst design has been required to achieve the reasonable efficiency.Here, we will present syntheses and characterizations of a series of cobalt complexes supported by a newly designed anionic PNP ligand (PNP^- = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide). A dinuclear cobalt(I) dinitrogen species {(PNP)Co}2(μ-N2) was generated from the chemical reduction of (PNP)CoBr revealing almost perfect square planar geometry about each cobalt center according to XRD data. By addition of H_2(g) and CO_2(g) sequentially to {(PNP)Co}2(μ-N_2), a cobalt monohydride species (PNP)CoH and cobalt formate species (PNP)Co(OCHO) were obtained with good yield. Under mild conditions for formate generation with {(PNP)Co}2(μ-N_2), the observed TOF of 1900 h^{-1} was obtained. Further investigations including the mechanism of formate generation will be discussed in detail.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-193**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Host-Guest Study of Matallacyclic Cage Containing two Bimetallic Schiff bases

허정석* <u>이인용</u>

충남대학교 화학과

Supramolecular cages are of great interest because of it has large potential applications such as gas separation, selective molecular recognition, chemical sensor, and catalyst based on Host-guest chemistry. Especially, bimetallic macrocyclic complexes have drawn chemists' attention because it has superior catalytic activities compared with monometallic metal complexes. We synthesized new type of bis-bimetallic cage compound by employing a bimetallic macrocycle as molecular a building block to embed binding site to the macrocyclic cage for guest molecule and as a catalytic active site. This cage has large pore size (15.920 Å * 3.77 Å) and two bimetallic centers as binding sites to guest molecule. We investigated binding study of the cage with many organic molecules. In poster session, detailed host-guest chemistry data will be presented.

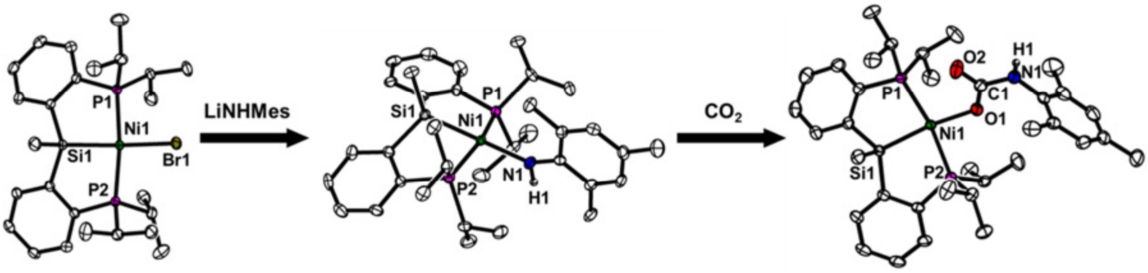
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-194**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of a Four-coordinate Nickel Carbamato Species (MeSiP2)Ni(OC(O)NHMes)

김진 이윤호*

KAIST 화학과

Carbon dioxide is not only a primary greenhouse gas, but also a natural abundant carbon source. Inspired by a biological enzyme, carbon monoxide dehydrogenase (CODH), several nickel complexes and their reactivity towards CO_2 have been investigated. However, limited studies have been reported for the transformation of carbon dioxide to carbamates mediated by nickel amido species. To investigate CO_2 reaction of the nickel amido species, $(MeSiP_2)Ni(NHMes)$ ($\mathbf{2}^{\mathbf{Mes}}$, Mes = 2,4,6-trimethylphenyl) and $(MeSiP_2)Ni(NHTrip)$ ($\mathbf{2}^{\mathbf{Trip}}$, Trip = 2,4,6-triisopropylphenyl) supported by a pincer type $MeSiP_2$ ligand ($MeSiP_2$ = $MeSi(2\text{-}P\mathit{i}Pr_2C_6H_4)_2^-$) were generated from the reaction of a nickel bromide complex $(MeSiP_2)NiBr$ (1) with lithiated arylamines. The nickel amido complex $\mathbf{2}^{\mathbf{Mes}}$ is fairly stable even at high temperature, while $\mathbf{2}^{\mathbf{Trip}}$ reveals a ligand rearrangement at room temperature in a solution state, resulting in a formation of $(\kappa^2\text{–}Cy_2PC_6H_4SiMe_2)Ni(\kappa^2\text{–}Cy_2PC_6H_4)$ ($\mathbf{3}^{\mathbf{Trip}}$). From an instantaneous reaction of $\mathbf{2}^{\mathbf{Mes}}$ with CO_2, a four coordinate nickel(II) carbamato complex $(MeSiP_2)Ni(OC(O)NHMes)$ (4) was successfully synthesized via an insertion process of CO_2 into a Ni–N bond. Compared to the formation of 4, a nickel(II) carbonato species $\{(MeSiOPP^O)Ni\}_2\text{-}\mu\text{-}CO_3\text{-}\kappa^2O,O$ (5, $MeSiOPP^O$ = $MeSiO(2\text{-}P\mathit{i}Pr_2\text{-}C_6H_4)(2\text{-}OP\mathit{i}Pr_2\text{-}C_6H_4)^-$) was generated from the reaction of $\mathbf{2}^{\mathbf{Mes}}$ with CO_2 under aerobic conditions. The syntheses of nickel complexes and their characterizations by various spectroscopic techniques and X-ray crystallography will be discussed.


P1
Ni1
Si1
Br1
P2
LiNHMes
Si1
P1
Ni1
N1
H1
P2
CO₂
O2
H1
N1
P1
C1
O1
Ni1
Si1
P2

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-195**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoinduced long-lived charge separation by self-assembled molecular p/n junctions on the indium tin oxide nanoparticle surface

배건오 위경량[1,*]

*대구대학교 화학*응용화학과 [1]대구대학교 화학응용화학과*

The achievement of long-lived photoinduced redox separation lifetimes has long been a central goal of molecular-based solar energy conversion strategies. The longer the redox-separation lifetime, the more time available for useful work to be extracted from the absorbed photon energy. Here we describe a novel strategy for dye-sensitized solar energy applications in which redox-separated lifetimes on the order of milliseconds to seconds can be achieved based on a simple toolkit of molecular components. Specifically, molecular chromophores (C), electron acceptors (A) and electron donors (D) were self-assembled on the surfaces of mesoporous, transparent conducting indium tin oxide nanoparticle (nanoITO) electrodes to prepare both photoanode (nanoITO|–A–C–D) and photocathode (nanoITO|–D–C–A) assemblies. Nanosecond transientabsorption and steady-state photolysis measurements show that the electrodes function microscopically as molecular analogues of semiconductor p/n junctions. These results point to a new chemical strategy for dye-sensitized solar energy conversion based on molecular excited states and electron acceptors/donors on the surfaces of transparent conducting oxide nanoparticle electrodes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-196**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Stabilization of Ruthenium(II) Polypyridyl Complexes on Nanoparticle Metal-Oxide Surface in Water by Hydrophobic Polymer Overlayers

이경민 위경량*

대구대학교 화학응용화학과

We describe a polymer dip-coating procedure, which results in surface stabilization of phosphonate and carboxylate derivatives of Ru(II)-polypyridyl complexes surface-bound to mesoporous nanoparticle TiO2 and nanoITO films in aqueous solutions. As shown by contact angle and transmission electron microscopy (TEM) measurements, rigid polymers conformally coat the metal-oxide nanoparticles changing the mesoporous films from hydrophilic to hydrophobic. The thickness of the PMMA overlayer on TiO2−Ru(II) can be controlled by changing the wt % of polymer in the dipcoating solution. There are insignificant perturbations in electrochemical or spectral properties at thicknesses of up to 2.1 nm with the Ru(III/II) couple remaining electrochemically reversible and E1/2 values and current densities nearly unaffected. Surface binding by polymer overlayers results in stable surface binding even at pH 12 with up to a ～100-fold enhancement in photostability. As shown by transient absorption measurements, the MLCT excited state(s) of phosphonate derivatized [Ru(bpy)2((4,4′-(OH)2PO)2bpy)]2+ undergo efficient injection and back electron transfer with pH independent kinetics characteristic of the local pH in the initial loading solution.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-197**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Unprecedented Supramolecular Architectures from the Self-Assembly of Tetrapyridyl Metalloligand Donor and Arene Ruthenium Acceptors

류지연 위은혜 이지민 박형련 이준승*

전남대학교 화학과

Two metal sandwich complexes, $[Cp^*Fe(\eta^4\text{-}C_4Py_4)]$ and $[CpCo(\eta^4\text{-}C_4Py_4)]$, were designed containing tetratopic pyridyl sites as connectors for self-assembly. As shown by X-ray crystal structures, cyclobutadiene ring ($\eta^4\text{-}C_4Py_4$) has square geometry and also parallel with cyclopentadienyl rings. This geometry makes the system an ideal coordinating metalloligand for self-assembly process. Reactions between these sandwich complexes with 4-pyridyl group as donors and different Ru-linkers, led to generate supramolecular cages via coordination-driven self-assembly. From X-ray crystallographic study, it is found that architectures were controlled in three different manners, depending upon the pi-pi interaction of donors with acceptors. The formation of self-assembled adducts in solution were further confirmed by ^{1}H-NMR spectroscopy, electrospray ionization mass spectrometry, in accordance with the solid structures.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-198**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

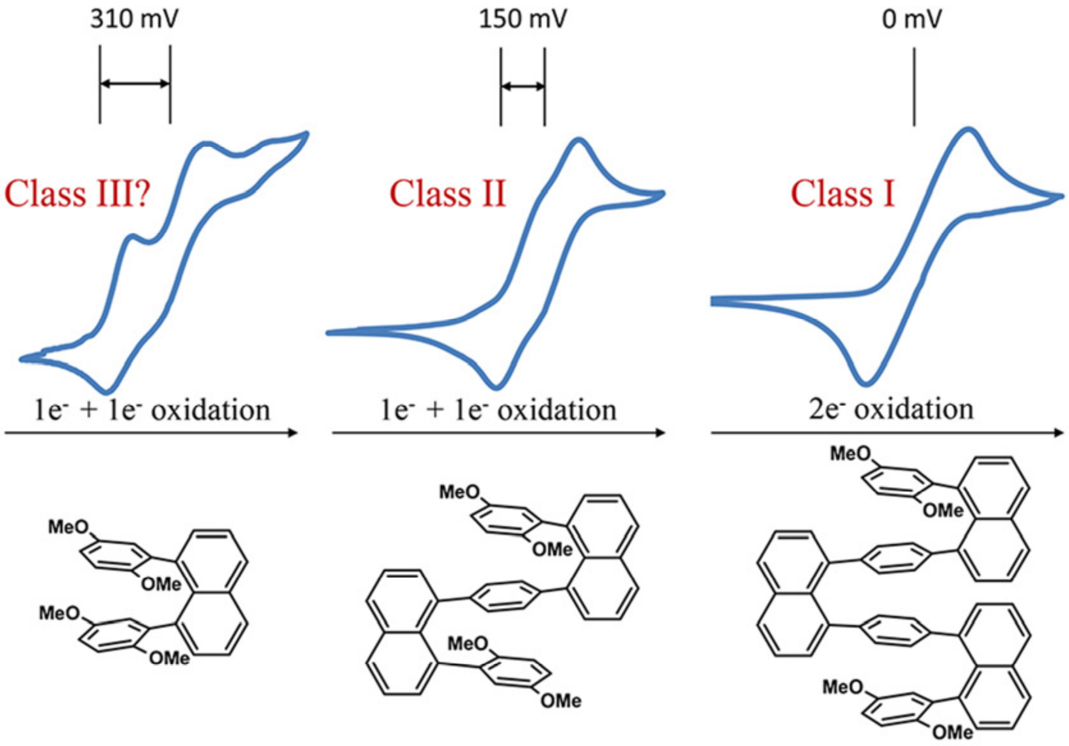
Organic mixed-valence system: Rigid, cofacially compressed,π-stacked dimethoxybenzenes with phenylene spacer(s) and naphthalene pillar(s)

윤성은 강윤경*

상명대학교 화학과

Electronic couplings mediated by series π-stacked aromatic components were evaluated in the organic mixed-valence cation radical $D\text{-}(ph)_n\text{-}D^{+\cdot}$ systems, where D = 2,5-dimethoxyphenyl, ph = phenyl, and n = 0 (1), 1 (2), and 2 (3). A 1,8-naphthyl pillaring motif can be utilized to enforce sub van der Waals interplanar separations between juxtaposed D and phenylene components. Such structures, synthesized via metal-mediated cross-coupling of appropriately functionalized precursors, manifest unusual conformational rigidity in the condensed phase, and varying degrees of electronic couplings between the cofacially aligned D components. Geometrical structure of neutral D-ph-D (2) compound was determined by X-ray crystallography while those of D-D (1) and $D\text{-}(ph)_2\text{-}D$ (3) as well as 1^+, 2^+, and 3^+ were obtained by DFT calculations. Optical and electrochemical methods were employed for the experimental measure of electronic coupling values. These experiments demonstrate that two degenerate states of $D\text{-}(ph)_n\text{-}D^{+\cdot}$ and $D^{+\cdot}\text{-}(ph)_n\text{-}D$ has no electronic coupling when n = 2 but has significant one with n = 1. Without phenylene spacer, the electronic coupling value reaches to the borderline between class II and class III of Robin and Day classification.

Organic Mixed Valence Compounds



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-199**

발표분야: 무기화학

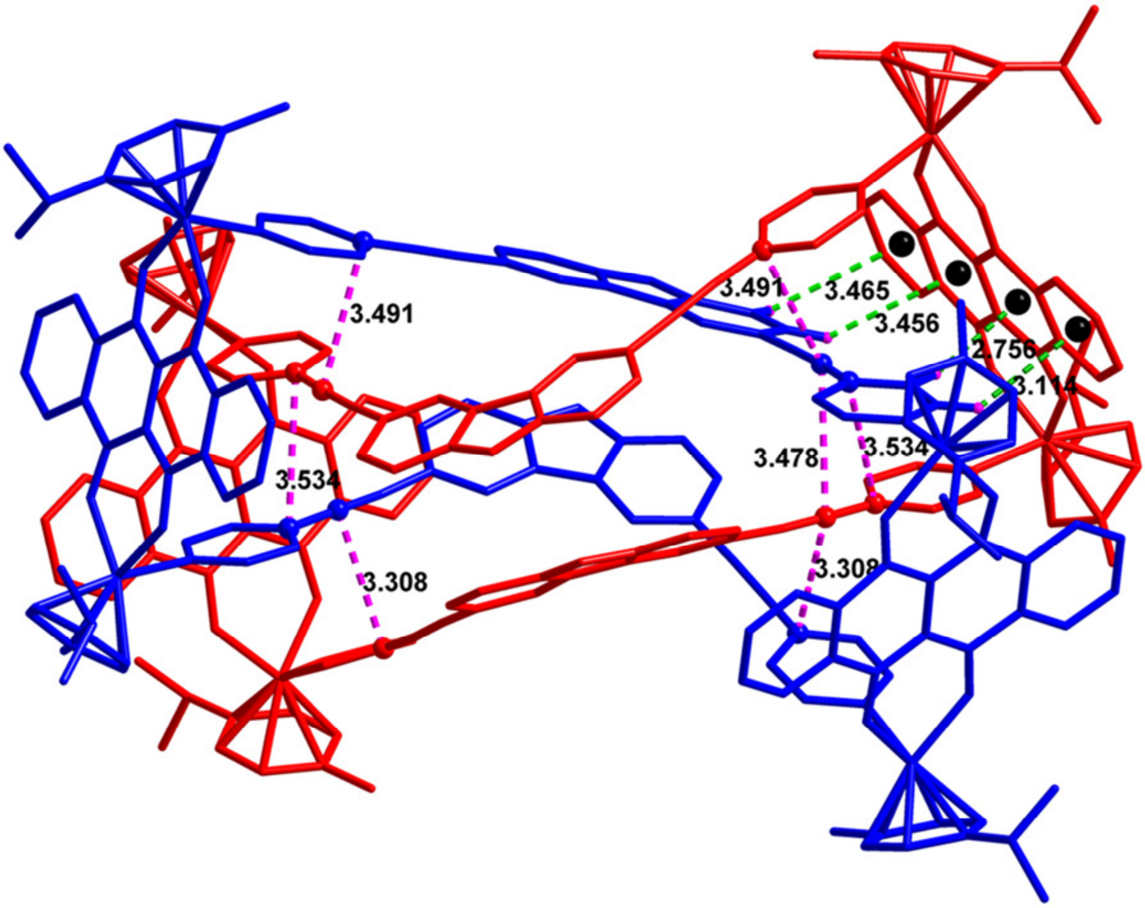
발표종류: 포스터, 발표일시: 목 11:00~12:30

Template-Free Synthesis of a Molecular Solomon Link by Two-Component Self-Assembly

SINGH NEM 김동환 지기환*

울산대학교 화학과

The topologically intriguing threaded molecular architectures such as catenanes,[1] trefoil, and pentafoil knots, Solomon links (a doubly-interlocked [2]catenane)[2], and Borromean rings[3] have attracted a great deal of attention not only because of their aesthetic charm but also because of their potential applications in nanomaterials, biomaterials, molecular machines, electronic devices, and sensors. Present work demonstrates the high yield synthesis of a molecular Solomon link through the template-free, coordination-driven self-assembly of a carbazole-functionalized donor and a tetracene-based dinuclear ruthenium(II) acceptor.[2] The doubly interlocked topology was realized by a strategically chosen ligand which was capable of participating in multiple CH···π and π–π interactions, as evidenced from single-crystal X-ray analysis and computational studies. This method is the first example of a two-component self-assembly of a molecular Solomon link using a directional bonding approach.References1. Lee, H.; Elumalai, P.; Singh, N.; Kim, H.; Lee, S. U.; Chi, K.-W. J. Am. Chem. Soc. 2015, 137, 4674.2. Song, Y. H.; Singh, N.; Jung, J.; Kim, H.; Kim, E.-H.; Cheong, H.-K.; Kim, Y.; Chi, K.-W. Angew. Chem. Int. Ed. 2016, 55, 2007. 3. Kim, T.; Singh, N.; Oh, J.; Kim, E.-H.; Jung, J.; Kim, H.; Chi, K.-W. J. Am. Chem. Soc. 2016, 138, 8368.


3.491
3.534
3.308
3.491
3.465
3.456
2.756
3.114
3.478
3.534
3.308

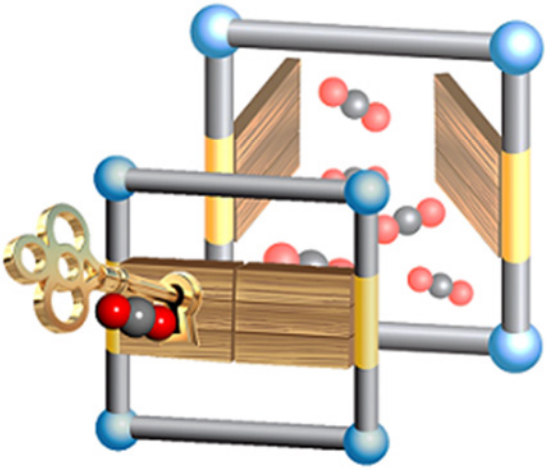
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-200**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Exploration of Gate-Opening and Breathing Phenomena in a Tailored Flexible Metal−Organic Framework

이재화 문회리*

UNIST 화학과

Flexible metal−organic frameworks (MOFs) show the structural transition phenomena, gate opening and breathing, upon the input of external stimuli. These phenomena have significant implications in their adsorptive applications. In this work, we report a well-designed flexible MOF at the synthesis stage, which shows both the gate-opening and breathing effects upon CO_2 adsorption. The structural information before and after structural arrangements are successfully provided by the X-ray powder diffraction (XRPD) and single-crystal diffraction (SCD) results, which enable the capture of the snapshots of the gate-opening and breathing phenomena. In addition, during the CO_2 adsorption, the specific sites in the flexible MOF that interact with CO_2 molecules to open the gate are verified by computational studies of multiscale simulations that are a combination of the density functional theory (DFT), molecular dynamics (MD), and grand canonical Monte Carlo (GCMC) simulations. This is the first study which elucidates the framework flexibility in the entire responsive process upon CO_2 molecules, before and after as well as during adsorption.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-201**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tetraphenylenethene-based three-dimensional metal-organic framework for chemical sensing

이한글 송정화 이종현 홍창섭*

고려대학교 화학과

We synthesized a [$Cd_3(ETTC)_{1.5}(H_2O)_2(DMF)$] (1) using the TPE-based ligand H_4ETTC [= 4’,4’’’,4’’’’’,4’’’’’’’-(ethane-1,1,2,2,tetrayl)tetrakis(1,1’-biphenyl-4-carboxylic acid)] via solvothermal reaction which exhibits three dimensional framework. In 1, Cd ions are bridged by oxygen atoms from DMF molecule and carboxylate groups to form a chain. This complex exhibits very strong fluorescence properties. The observed fluorescence properties could benefit potential applications in chemical sensor. Detailed structural characterizations and other physical properties will be given in the presentation.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-202**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, crystal structure and sensing properties of a 2D cadmium framework with an oxidized ligand

이종현 송정화 이한글 홍창섭*

고려대학교 화학과

We have synthesized a two-dimensional coordination polymer $[Cd_3(DSBDC)_{1.5}(DMF)_6]$ (1) ($DSBDC^{2-}$ =2,5-disulfo-1,4-benzenedicarboxylate) using a solvothermal reaction of $Cd(NO_3)_2{\cdot}4H_2O$ and H_2DMBDC (2,5-dimercapto-1,4-benzenedicarboxylic acid) as an organic linker in DMF solvent. Thiol group in ligand was oxidized to sulfonic acid groups during the reaction. Compound 1 crystallizes in the monoclinic system with the space group C2(1)/c. It contains three Cd^{2+} ion, one and half DSBDC ligand and six DMF molecules. Each Cd^{2+} ion is coordinated by six oxygen atoms from four DSBDC ligands and two oxygen atoms from DMF molecules. Compound 1 was characterized by PXRD, IR, elemental analysis and single crystal X-ray diffraction. This compound shows highly selective sensing of nitrobenzene (NB), which could be quenched by trace amounts via fluorescence quenching mechanism. Detailed structures and other measurements will be given in the presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-203**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structural transformations and conductivity changes in Zn coordination complexes depending on relative humidity conditions

송정화 이종현 이한글 홍창섭*

고려대학교 화학과

We prepared three types of Zn-based coordination systems $[Zn(H_2SSA)_2(H_2O)_2]$ (1), $[Zn(H_2O)_6]\cdot 2(H_2SSA)\cdot 2(H_2O)$ (2) and $[Zn(H_2O)_6]\cdot 2(H_2SSA)\cdot 4(H_2O)$ (3) using the H_3SSA ligand (H_3SSA=5-sulfosalicylic acid) via solvothermal synthesis. Compound 1 exhibits structural transformations and considerable changes in proton conduction properties under different relative humidity conditions. To elucidate the structural change process, we characterized each phase as temperature and humidity vary. Detailed characterizations and proton conduction studies will be given in the presentation.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-204**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Study of Highly Stable Metal Organic Framework (MOF) as Photosensitizer for Carbon Dioxide Reduction

정원조 이종수 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

화석연료의 사용량 증가로 인한 CO_2 발생량의 폭발적인 증가로 인하여 지구온난화와 기후변화로 기인된 자연폐해가 가속화 됨에 따라 전세계적으로 CO_2 저감 및 활용을 위한 연구개발에 많은 투자가 이루어지고 있는 상황이다. 많은 관련 기술 중 가시광을 이용하여 CO_2 환원반응의 유도를 위한 방법으로 태양빛을 이용한 청정공정연구가 각광받고 있다. 최근에는 Metal Organic Framework (MOF)의 안정성을 토대로 CO_2 환원에 적용한 연구가 진행되고 있다. 이에 본 연구에서 photosensitizer 로 zinc-porphyrin 기반의 MOF 인 Zirconium-Metalloporphyrin PCN-222 를 사용하고 TiO_2에 anchoring 하기 위한 방법으로서 –COOH, -PO_3H_2 group 이 치환된 rhenium catalyst 를 사용하였으며 장수명의 hybrid binary system (PCN-222+TiO_2/ReC)을 구현하고자 하였다. 또한 CO_2 전환 효율을 높이기 위해 PCN-222 에 Atomic Layer Deposition (ALD) 처리를 하여 측정하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-205**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and application of [(Bpy-mPH)M(CO)$_3$X, M=Mn, Re, X=Cl, Br] Complexes in Photocatalytic CO$_2$ Reduction

우성준 정원조 강상욱[1] 손호진[*]

고려대학교 신소재화학과 [1]고려대학교 소재화학과

본 연구에서는 같은 리간드를 다른 중심금속 (Mn 또는 Re)에 배위시켜 비슷한 유기금속 화합물 두 종을 합성 및 분석 하였다. 이 화합물을 광화학적 이산화탄소 환원에 적용시켜 더 값싸고 양이 많은 Manganese 로 Rhenium 을 대체할 수 있는 가능성을 알아보기 위한 실험을 진행 하였다. 기본적인 실험 과정으로는 이전 연구에서 주목 받은 Ternary system (Dye/TiO$_2$/Catalyst)을 적용하였고, 광원으로 가시광 영역의 LED 를 사용하였으며, 교반장치로는 Merry-go-round 시스템을 사용하였다. 광반응 용매로는 CO$_2$ 용해도가 높은 DMF 를 이용하였고, 전자주개로 BIH 를 이용하였다. 가시광 영역인 ≥420 nm 빛을 조사하였을 때, 촉매 메커니즘은 유기염료가 광자를 흡수하여 들뜬 전자들이 TiO$_2$ 의 conduction band 로 이동되고 그 전자들이 최종적으로 유기금속 화합물 위치로 이동하여 CO$_2$ 가 환원되는 것이다. 광반응을 실행 하였을 때 중심 금속이 달라짐에 따라 주요 CO$_2$ reduction 생성물의 종류 및 효율의 차이를 확인할 수 있었다. Re(I)이 중심이 된 촉매의 경우 주요생성물인 CO 가 150 의 turnover number (TON)을 나타낸 반면, 중심금속이 Mn 의 경우 Formic acid 가 주요 생성물로서 50 시간 동안 300 의 TON 값을 나타내었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-206**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photochemical CO_2 Reduction using Butadiyne-linked Porphyrin Trimers and Dimers as Sensitizer in Binary System (Dye + TiO_2/Catalyst)

최성한 우성준 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

Efficient and selective photoreduction of CO_2 to deeply reduced products such as hydrocarbons is a big challenge. We use the porphyrin as sensitizer to enhance the electron charge injection to TiO_2. For CO_2 reduction system, Butadiyne-linked porphyrin trimers and dimers were synthesized and investigated. Herein we adapted the porphyrin trimer and dimer to binary system (Dye + TiO_2/Catalyst). The system comprises [[5,5’'-(1,3-Butyne-1,4-biyl)bis[10,20-bis[2,6-bis[di(n-hexoxy)]phenyl]]-15[(triisopropyl)ethynyl]-porphin-5-yl]-1,3-butadiynyl]-10,20-bis[2,6-bis[di(n-hexoxy)]phenyl]-porphinato]trizinc as the sensitizer and (4,4′-bis(methylphosphonic acid)-2,2′-bipyridine)$Re^{I}(CO)_3Cl$ as the catalyst, which have been anchored on TiO_2 nanoparticle. It was found that remarkable enhancements in the CO_2 conversion activity of the hybrid photocatalytic system can be achieved by using the porphyrin trimer than monomer.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-207**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Widely Controllable Syngas (H_2 + CO) Production by a Dye-Sensitized TiO_2 Hybrid System with Re(I) and Co(III) Dual Molecular Catalysts under Visible-Light Irradiation

이종수 최성한 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

Visible-light irradiation of a ternary hybrid catalyst prepared by grafting a dye, an H_2 evolving Co(III) catalyst and a CO-producing Re(I) catalyst has been found to produce both H_2 and CO (syngas) in CO_2-saturated DMF/water solution. The H_2/CO ratios are effectively controlled by changing either the water content in solvent or the molar ratio of the two Re(I) and Co(III) catalysts, being ranged from 1:2 to 16:1. The syngas formation with controlled H_2/CO ratios has been discussed in terms of competitive electron flow from TiO_2 to the CO_2-reduction site and to the hydrogen-evolving site depending on the flat-band potential shifts of TiO_2 induced by water

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-208**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular design of squaraine dyes for efficient far-red and near-IR sensitization in CO_2 reduction

최성한 우성준 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

본 연구에서는 TiO_2 반도체에 흡광체인 유기염료와 CO_2 환원촉매를 흡착시킨 triad 광반응 시스템 (Dye/TiO_2/Catalyst)을 이용하여 CO_2 를 CO 로 환원하는 연구가 진행되었다. Triad 광반응 시스템에 ≥420 nm 빛을 조사하면 유기염료가 빛을 흡수하여 들뜨고, 들뜬 전자들이 TiO_2 의 conduction band 를 통해 CO_2 환원 촉매로 이동하여 CO_2 가 CO 로 환원되는 것에 사용된다. 광반응 후 유기염료에서 생성되는 radical cation 은 전자 주개 (ED)인 BIH 에 의해 환원되며, ED 로 부터 재생된 염료는 다시 빛을 흡수하여 광반응 시스템에 이용된다. 이를 기반으로 낮은 에너지인 Near-IR (700 nm)을 흡수하는 Squaraine 염료를 흡광체로 사용하여 높은 효율을 기대하였다. 또한 TiO_2 로부터 흡광체의 탈착을 막기위해 Atomic Layer Deposition (ALD)의 공정을 사용하였고, ALD 공정 횟수에 따른 TiO_2 layer 의 두께 차이 별로 광반응 전환효율을 비교하였다. 정확한 메커니즘 분석을 위해 광물리적 그리고 전기화학적 특성이 분석되었고, 광반응을 통하여 Squaraine 염료들이 흡착된 광촉매 시스템의 전환효율이 평가 되었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-209**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Role of Porphyrin Antenna for Photocatalytic CO_2 Reduction in a Hybrid Catalyst System: Protection from Photo-bleaching

우성준 정원조 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

Porphyrin dye was chosen for the test of nature’s best adapted photosynthetic dye, Chloropyll. The long-term test of photocatalytic reaction clearly shows that the increase of anchoring ability of porphyrin molecules and the utilization of low energy as light source directly relates to the steady performance on the photocatalytic CO_2 reduction. Thus, a series of visible light harvesting porphyrin antenna have been engaged to the hybrid photocatalyst system for CO_2 reduction and recorded unprecedented catalytic performance within a range of ~1,000 TON for 40h with its highly enhanced durability under low-energy light conditions.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-210**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Photosensitization Effects of Ir(III) Complexes in Selective Reduction of CO_2 by Re(I)-Complex-Anchored TiO_2 Hybrid Catalyst

이종수 최성한 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

A series of cationic Ir(III) complexes ($[Ir(btp)_2(bpy\text{-}X_2)]^+$ (Ir-X^+): btp = (2-pyridyl)benzo[b]thiophen-3-yl; bpy-X_2 = 4,4'-X_2-2,2'-bipyridine (X = OMe, ^{t}Bu, Me, H, and CN)) were applied as visible-light photosensitizer in solution to the selective CO_2 reduction to CO in the presence of an electron donor (BIH) and a hybrid catalyst (TiO_2/ReC) prepared by anchoring of Re(4,4'-Y_2-bpy)$(CO)_3$Cl (Y = $CH_2PO(OH)_2$) on TiO_2 particles. Irradiation of the system in N,N-dimethylformamide (DMF) at > 400 nm resulted in the successful reduction of CO_2 to CO with efficiencies in the order X = OMe > ^{t}Bu ~ Me > H; Ir-CN+ has no photosensitization effect. An interesting observation is that Ir-^{t}Bu$^+$ and Ir-Me$^+$ are less efficient than Ir-OMe$^+$ at an early stage of the reaction but reveal persistent photosensitization behavior for a longer period of time unlike the latter. Comparable experiments showed that (1) the Ir-X^+ sensitizers are commonly superior compared to $Ru(bpy)_3^{2+}$, a widely used transition-metal photosensitizer, and (2) the system comprising Ir-OMe$^+$ and TiO_2/ReC is much more efficient than a homogeneous-solution system using Ir-OMe$^+$ and Re(4,4'-Y'_2-bpy)$(CO)_3$Cl (Y′ = $CH_2PO(OEt)_2$). Implications of the present observations and reaction mechanisms are discussed in detail

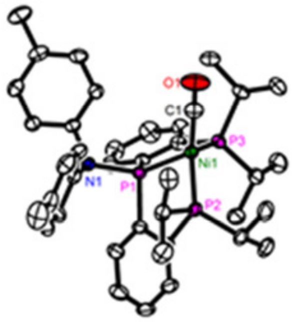
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-211**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

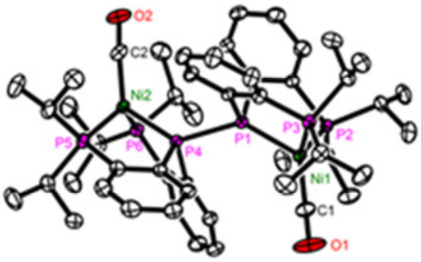
Uncommon Metal-Ligand Cooperation on a (PPP)Ni Scaffold via Reversible P-P Bond Coupling

김영은 이윤호*

KAIST 화학과

Metal-ligand cooperation continues to attract attention. Since a ligand can deliver electron(s), a proton and/or even a functional group to assist the chemistry at a metal center, metal-ligand cooperation can be utilized as a new synthetic methodology to extend the role of transition metal ions in multi-electron catalytic reactions. Several examples which employ redox noninnocent ligands were reported to transfer electron(s) through a ligand system. Aromatization/ dearomatization is also considered as metal-ligand cooperation to carry a proton via employing pyridine- or acridine-based pincer ligand. Recently, our group reported a new type of metal-ligand cooperation with an anionic PPP ligand (PPP^- = $^-P[2\text{-}P\textit{i}Pr_2\text{-}C_6H_4]_2$). The reversible phosphide/phosphinite interconversion of a PPP ligand coupled with a 2-electron redox change of nickel (II and 0) was observed in this system. Here, reversible formation of P-N and P-P bonds at a nickel center supported by a PPP ligand will be presented. Two different types of divalent nickel amide species with amido groups (-NHMes and –$NTol_2$) shows the different reactivity toward CO. While the formation of a P-N bond was successfully accomplished by addition of CO(g) to the solution of (PPP)Ni-$NTol_2$ (Figure, left), the formation of a dimeric nickel(0) species, $\{(PPP)NiCO\}_2$ was observed from the reaction of (PPP)Ni(NHMes) with CO(g) (Figure, right). P-P bond cleavage was accomplished by further reaction of $\{(PPP)NiCO\}_2$ with H_2 to give $(PP^HP)NiCO$. Further reactivity toward various reagents to activate P-N and P-P bonds will be discussed in this poster.


O1
C1
P3
Ni1
N1
P1
P2


O2
C2
Ni2
P5
P6
P4
P1
P3
P2
Ni1
C1
O1

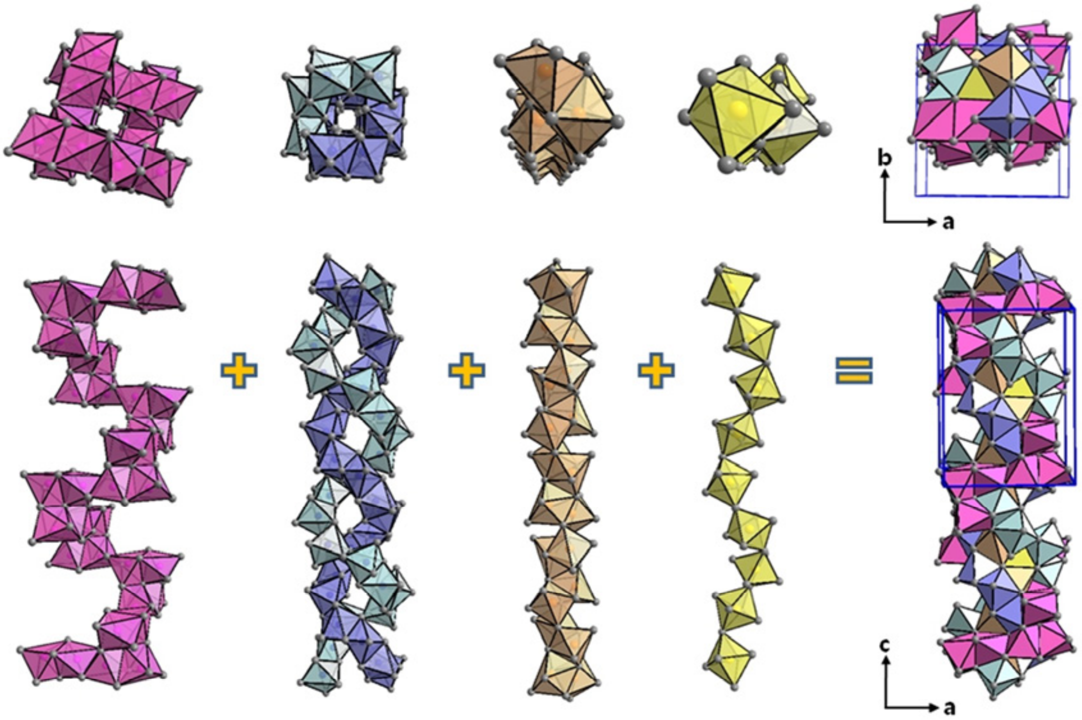
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-212**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cationic Site-Preference in the $Yb_{14-x}Ca_xAlSb_{11}$ ($4.81 \le x \le 10.57$) Series: Theoretical and Experimental Studies

남근우 유태수*

충북대학교 화학과

Four quaternary Zintl phases with mixed-cations in the $Yb_{14-x}Ca_xAlSb_{11}$ ($4.81 \le x \le 10.57$) series have been synthesized by using the arc-melting and the Sn metal-flux reaction methods, and isotypic crystal structures of the title compounds have been characterized by both PXRD and SXRD analyses. The overall crystal structure adopting the $Ca_{14}AlSb_{11}$-type can be described as a pack of four different types of the spiral-shaped 1-dimensional octahedra chains with various turning radii, each of which is formed by the distorted $[(Yb/Ca)Sb_6]$ octahedra. Four symmetrically independent cationic sites contain mixed-occupations of Yb^{2+} and Ca^{2+} with different mixing ratios and display a particular site-preference by two cationic elements. Two hypothetical structural models of $Yb_4Ca_{10}AlSb_{11}$ with different cationic arrangements were designed and exploited to study the details of site- and bond-energies. QVAL values provided the rationale for the observed site-preference based upon the electronegativity of each atom. Density of states (DOS) curves indicated a semiconducting property of title compounds, and crystal orbital Hamilton population (COHP) plots explained individual chemical bonding between components. Thermal conductivity measurement was performed for $Yb_{8.42(4)}Ca_{5.58}AlSb_{11}$, and the result was compared with compounds without mixed-cations.



(a) *M*1 (b) *M*2 (c) *M*3 (d) *M*4 (e) *M*1 + *M*2 + *M*3 + *M*4

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-213**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The n-doping effect for the thermoelectric property of the $Eu_{11}SnBi_{9-x}Te_{x}$($x = 0.4, 0.6$) series: Experimental and Theoretical Studies

유태수* 최웅진 이준수

충북대학교 화학과

Two title compounds have been synthesized by using high temperature synthetic method in a Nb ampule and characterized by powder and single crystal X-ray diffractions. Both compounds crystallized in the tetragonal $Ho_{11}Ge_{10}$-type structure (space group $I4/mmm$, Pearson symbol *tI*84). A series of theoretical calculations using tight-binding linear muffin-tin orbital (TB-LMTO) method were also performed to understand chemical bonding and the overall electronic structure. The compounds adopting the $Ho_{11}Ge_{10}$-type structure are known to show promising properties as thermoelectric materials, such as significantly reduced thermal conductivity caused descended from a complex crystal structure and the comparable electrical conductivity. However, due to the compensation effect between holes and electrons in the compounds, some of those candidate compounds display relatively low Seebeck coefficients. In order to figure this issue out, we have attempted to introduce the electron doping on the title compounds to produce the n-type TE materials. According to the SXRD experiments, there exists a site-preference among anionic elements. anionic elements indicate the particular site preference, which can be understood by using the atomic site of volume. It can expect that the smaller atomic site volume should occupy the smaller atom. Thus, the covalent radius of Te element lower than Bi element occupies at *Wyckoff* 8*j* site the smallest site volume among three anionic sites.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-214**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Experimental and Theoretical Investigations for the p-doping Effects on the$Eu_{11-x}M_xSnBi_9$(M = Li, Ca; x = 1, 3) Series

최웅진 이준수 유태수*

충북대학교 화학과

Total four title compounds in the $Eu_{11-x}M_xSnBi_9$ series (M = Li, Ca; x = 1, 3) have been synthesized by the high temperature synthetic method using a Nb-tube and characterized by powder and single crystal X-ray diffractions (PXRD, SXRD). All compounds crystallized in the isotypic crystal structure of the $Ho_{11}Ge_{10}$-type (tetragonal space group *I*4/*mmm*, Pearson symbol *tI*84) with nine crystallographically independent atomic sites in each unit cell. The series of compounds adopting the $Ho_{11}Ge_{10}$-type structure have been known for their promising thermoelectric properties, such as the significantly reduced thermal conductivity caused by complex crystal structures and the relatively high electrical conductivities. However, due to the compensation effect between holes and electrons co-existing in the same compound, some of those promising candidates display unexpectedly low Seebeck coefficients. To improve this property, we attempted to introduce the hole-doping on the title compounds to produce the p-type thermoelectric materials. According to the SXRD results, there exist the site-preference among cationic elements, and this observation can be understood based upon the quantity called QVAL values.

A series of theoretical calculations using tight-binding linear muffin-tin orbital (TB-LMTO) method was also performed to understand the overall electronic structures including QVAL values. These values can be evaluated from the calculations, and the values imply that the element having the higher electronegativity should occupy the atomic site with the larger QVAL value. Therefore, in the title compounds, since the electronegativity of Li or Ca is lower than that of Eu, Eu should occupy the *Wyckoff* 8*h* site having the smallest QVAL value among four cationic sites.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-215**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Covalently Polymer-Grafted Metal-Organic Frameworks based Mixed-Matrix Membrane for Gas Separation

김진영 문회리[1,*]

UNIST 친환경에너지공학부 [1]UNIST 화학과

Membrane is one of most cost-effective candidates for gas separation, which can separate mixture continuously without regeneration. Metal Organic Frameworks (MOFs) are attractive material for the separation due to selective host-gas molecule interactions and high permeability, but their fragile nature limits membrane fabrication in large area. MOF Mixed Matrix Membranes (M^4) are promising class of membrane for gas separation because they have both advantages of MOFs and polymers, high selectivity of MOFs and high mechano-chemical stability and easy processability of polymer. However, inevitable voids are the major challenge in this area, which are resulted from poor interaction between MOF and matrix polymer and debase the performance of the membrane. Herein, a directly grafting co-polymerization strategy was introduced to grow covalently tethered polymer on MOF surface, thus unavoidable voids can be effectively reduced and interaction between MOF and polymer was improved. Detailed characterizations about covalent bond between MOF and polymer and improved interaction between MOF and matrix polymer were discussed in this presentation.

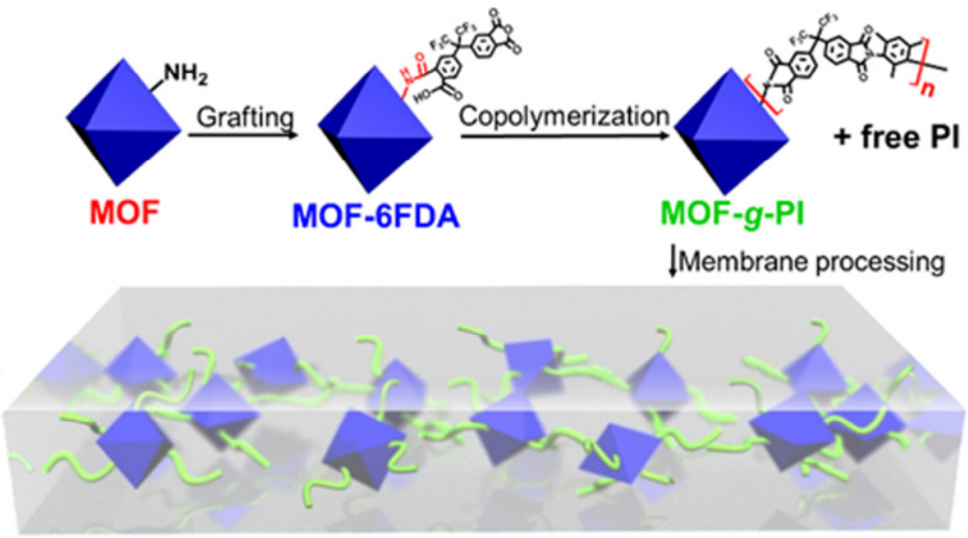


Figure 1. Schematic illustration of directly grafting co-polymerization and MOF-Mixed Matrix Membrane (M^4)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-216**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photo-Induced Reversible Transformations of Azobenzene-Incorporated Polyurea Thin Film Grown by Molecular Layer Deposition

김혜인 최의진 박이슬 이진석*

숙명여자대학교 화학과

Photo-sensitive polymer film has been attracted in the field of material science including biological system and optical devices which are sensitive on the change of surface topology. Recently, azo compound (R-N=N-R’), as one of the photo-induced reversible transformation unit, has been highlighted in the research related photo-sensitive polymer film including surface science, artificial muscle, biological and optical application, because light used as external triggers for inducing surface transformation is manageable to control without modification of nano-structures and environment concerns.In this study, we fabricated photo-reversible polyurea film based on coupling reactions between phenylenediisocyanate (PDI) and 4,4-diaminoazobenzene (AAB) by molecular layer deposition through self-limiting surface reaction, and investigated the photo-induced reversible transformation of azobenzene-incorporated polyurea thin film. In situ Fourier Transform Infrared (FTIR) measurement was used to monitor the growth of polyurea film, and the light-induced transformations of surface topography was characterized by Atomic Force Microscopy (AFM). Also, to measure the orientation of chemical bondings in azobenzene-incorporated polyurea film, plan-polarized grazing angle FTIR spectroscopy was used.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

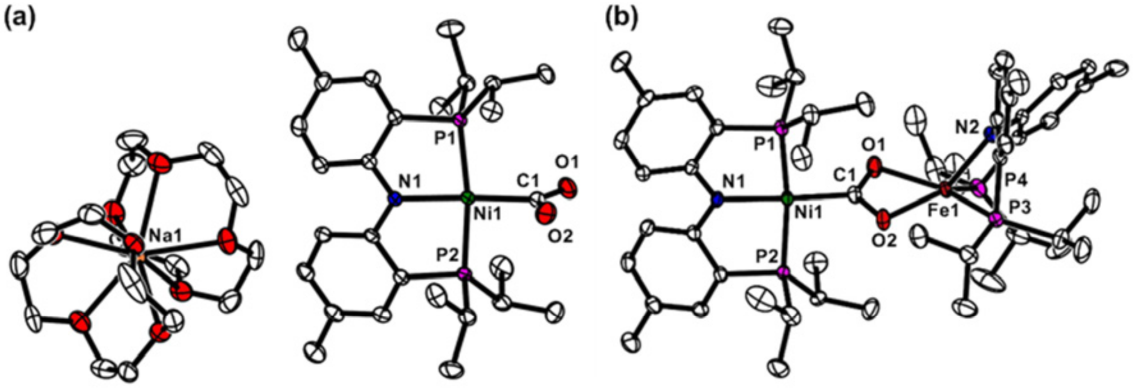
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-217**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

CO_2 coordination at a heterobimetallic Ni/Fe center

유창호 이윤호*

KAIST 화학과

Conversion of carbon dioxide has been one of the major research topics in recent years not only to contribute to find the solution for the global climate change and but also to recycle CO_2 as a cheap and abundant C1 source to produce useful chemicals and renewable fuels. Even with remarkable advances in the CO_2 reduction chemistry using transition metal complexes, their efficiencies and selectivity are limited to be utilized in chemical industry. In fact, an efficient catalytic conversion of CO_2 to CO occurs at the NiFe-bimetallic center in carbon monoxide dehydrogenase (CODH). Recent crystallographic studies show the structure of a CO_2^-bound species revealing the Ni-μ-COO-Fe fragment. Understanding of the interactions between a nickel ion and CO_2 in a coordination environment similar to that revealed in the CODH active site is of fundamental interest and crucial for the future development of efficient synthetic catalysts for CO_2 activation chemistry.Here we present a series of nickel carboxylate species supported by an anionic PNP ligand ($PNP^- = {}^-N[2\text{-}P^iPr_2\text{-}4\text{-}Me\text{-}C_6H_3]_2$). Mononucelar Ni-COOH (**1**) and $Ni\text{-}COO^-$ (**2**) species showing a η^1-κC mode, and dinuclear Ni-COO-M species (M = Ni (**3**) or Fe (**4**)) with a μ_2-κC:κO or μ_2-κC:κ^2O,O' binding mode were identified revealing a plausible binding mode of CO_2 at the active site of CODH. In particular, compound **4** is the first example of a heterobimetallic Ni-CO_2-Fe species, of which structural and electronic features are reminiscent to those of a Ni-μ-CO_2-Fe fragment found in CODH. The comparison of a η^1-CO_2-κC species **2** and a dinuclear Ni-μ-CO_2-Fe species **4** with previously reported Ni-CO_2 adducts suggests that a CO_2 ligand can be stabilized and activated by a second metal interaction. The protonation of Ni-CO_2 complexes results in C-O bond cleavage to produce $\{(PNP)Ni^{II}CO\}^+$ exhibiting the importance of a M-C bond in CO_2 conversion.


(a)
Na1
P1
O1
N1
C1
Ni1
O2
P2
(b)
P1
N1
O1
C1
Ni1
O2
P2
N2
P4
Fe1
P3

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-218**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation properties of GaN epitaxial layer on non-catalytically-grown graphene for lift-off

신현호 황성원[1,*]

건국대학교 의생명화학과 [1]건국대학교 나노전자기계공학과

Sapphire is widely used as a substrate for the growth of GaN epitaxial layer (EPI), but has several drawbacks such as high cost, large lattice mismatch, non-flexibility, and so on. Here, we first employ graphene directly grown on Si or sapphire substrate as a platform for the growth and lift-off of GaN-light-emitting-diode (LED) EPI, useful for not only recycling the substrate but also transferring the GaN-LED EPI to other flexible substrates. Sequential standard processes of nucleation/recrystallization of GaN seeds and deposition of undoped (u-) GaN/AlN buffer layer were done on graphene/substrate before the growth of GaN-LED EPI, accompanied by taping and lift-off of u-GaN/AlN or GaN-LED EPI. This approach can overcome the limitations by the catalytic growth and transfer of graphene, and make the oxygen-plasma treatment of graphene for the growth of GaN EPI unnecessary.Supported by Korea Evaluation Institute Of Industrial Technology (10067533), Republic of Korea

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-219**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Correlation between Thermoelectric Property and Metal to Semiconductor Transformation in the $Ca_{5-x}Yb_xAl_2Sb_6$ ($1.5 \le x \le 4.5$) Series

유태수* 남근우 최웅진 임성지

충북대학교 화학과

The $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 1.5-4.5) series have been synthesized using an arc-melting method. The structural analysis has been conducted based upon both powder and single crystal X-ray diffractions, and chemical compositions have been verified by the Energy dispersive X-ray spectroscopy. The orthorhombic $Ca_5Ga_2Sb_6$-type structure (space group *Pbam*, Pearson code *oP26*) was observed for the Ca-richer $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 1.5, 2) compounds, whereas the orthorhombic $Ba_5Al_2Bi_6$-type structure (space group *Pbam*, Pearson code *oP26*) was adopted by the Yb-richer $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 3-4.5) compounds. Interestingly, the current study reveals that, for the first time, the phase transition from the $Ba_5Al_2Bi_6$-type to the $Ca_5Ga_2Sb_6$-type structure can occur via the simple annealing process at 800 ℃, which results in the enhanced thermoelectric property. The crystal structures of both Ca-richer and Yb-richer $Ca_{5-x}Yb_xAl_2Sb_6$ ($Ca_5Ga_2Sb_6$- and $Ba_5Al_2Bi_6$-type, respectively) share some portions of structural similarities including the one-dimensional $[Al_2Sb_6]^{10-}$ double chain composed of the $[AlSb_4]$ tetrahedra, the connecting Sb_2 dimers and the space filling Yb^{2+} and Ca^{2+} cations. However, different spatial arrangement of the $[AlSb_4]$ tetrahedra and the Yb^{2+}/Ca^{2+} cations generates two given distinctive structure types. Electronic structures and chemical bonding were studied by using tight-binding linear muffin-tin orbital (TM-LMTO) method for a structural model of $Ca_{2.5}Yb_{2.5}Al_2Sb_6$. Density of states, crystal orbital Hamilton population and electron localization function were interrogated. Thermoelectric properties including electrical resistivity, Seebeck coefficient as well as thermal conductivity of the $Ca_{5-x}Yb_xAl_2Sb_6$ (x = 1.5, 3.5) series were thoroughly investigated. Lastly, the variations in thermoelectric properties caused by the structural transition were also discussed.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-220**

발표분야: 무기화학

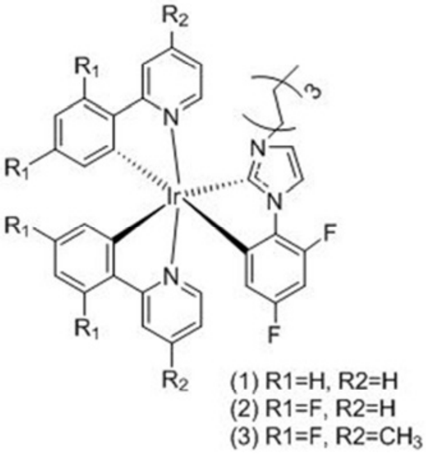
발표종류: 포스터, 발표일시: 목 11:00~12:30

Blue-green Phosphorescent Iridium(III) Complexes with Hexyl phenyl imidazole based Carbene Ligands for Organic Light-Emitting Diodes (OLEDs)

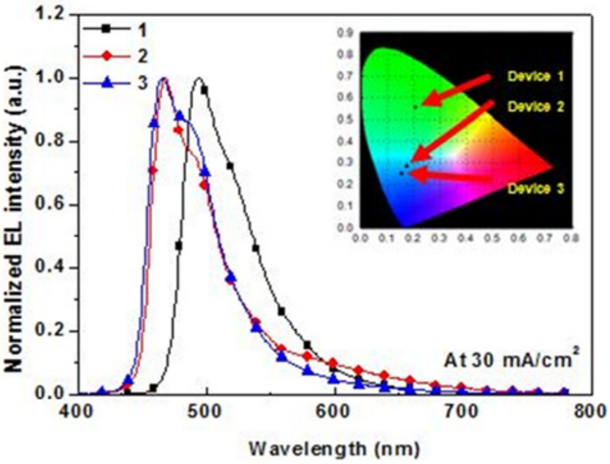
전진실 김영인* 최지혜 윤성재[1]

부산대학교 화학교육과 [1]한국원자력연구원 생명공학연구부

Cyclometalated iridium(III) complexes have been attracted broad attentions due to their high external quantum efficiency and color tunability, and applied for organic light-emitting devices (OLEDs). OLEDs have been developed and focused because of their applicability in solid-state lighting and full-color flat displays. In this study, we designed and synthesized heteroleptic cyclometalated Ir(III) complexes containing ppy-based main ligand and a hexyl phenyl imidazole based carbene ancillary ligand ; ppyIrdfimi (1), dfppyIrdfimi (2), dfpmpyIrdfimi (3) (2-phenylpyridine (ppy); 2-(2,4-diflorophenyl)pyridine (dfppy); 2-(2,4-diflorophnyl)-4-methylpyridine (dfpmpy); 1-(2,4difluorophenyl)-3-hexyl-1H-imidazol-3-ium (dfimi)). In addition, the photophysical, electrochemical and electroluminescent properties of complex (1), (2) and (3) were investigated. The phosphorescence properties of complex (1), (2) and (3) showed blue and green emission at 498, 468 and 465 nm in PL spectra with quantum yield of 70, 38 and 44 % in dichloromethane solution, respectively. The device performance of the iridium(III) complex 3 showed CIE coordinates of (0.15, 0.25), maximum external quantum efficiency of 6.37 %, luminance efficiency of 10.61 cd/A and turn on voltage of 3.57 V, showing that complex 3 a good candidate for blue OLED application.



(1) R1=H, R2=H
(2) R1=F, R2=H
(3) R1=F, R2=CH_3



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-221**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Multi-frequency, multi-technique EPR studies on high-valent cobalt complexes

김유정 고유경[1] 남원우[2] 김선희[3,*]

이화여자대학교 화학나노과학과 [1]한국기초과학지원연구원 분석연구부 [2]이화여자대학교 화학과 [3]한국기초과학지원연구원 서울서부센터

Notably, high-valent metal oxo species are suggested to mediate a plethora of vital oxidation reactions; C-H bond activation, sulfoxidation reaction, and water oxidation, for instance. Meanwhile, the “oxo wall” theory has proposed that cobalt complexes are rare or difficult to form terminal oxo compounds. Therefore, it is essential to verify the possibility of a cobalt complex to yield high-valent oxo species and illustrate its structure. Interestingly, high-valent cobalt oxo intermediate of Co(TAML) was successfully synthesized and the coordination geometry of Co(TAML) was characterized by Electron paramagnetic resonance(EPR) spectroscopy. Here, we use the X-band(9 GHz), the Q-band(34 GHz) and the W-band(94 GHz) EPR spectra of Co(TAML) to investigate its coordination structure. Q-band(34 GHz) electron nuclear double resonance (ENDOR), electron spin echo envelope modulation(ESEEM) and X-band hyperfine sublevel correlation(HYSCORE) experiments were carried out to examine metal-oxo species is formed by using an ^{17}O isotopically labeled one. Furthermore, Q-band ^{1}H ENDOR, ^{14}N ESEEM and X-band ^{14}N HYSCORE measurements were performed to explore geometrical structure of the complex. Overall, the structure of Co^{IV}(TAML)(O) was identified using multi-frequency and multi-technique EPR.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-222**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Elucidating Fibrilization Mechanism of Amyloid Peptides Relevant to Alzheimer's Disease; An EPR Study

홍수경 정한솔[1] 김선희[2,*]

이화여자대학교 자연대학 화학나노과학과 [1]이화여자대학교 화학나노과학과 [2]한국기초과학지원연구원 서울서부센터

Alzheimer's disease (AD) is a neurodegenerative disorder and AD has come to cause serious problems for both individuals and society. Interestingly, high concentration of copper ion has been found in the brain of Alzheimer's patients; thus, it has been suggested that copper ions affect aggregation of the Amyloid beta peptide (Aβ). However, there is no discrete knowledge about the fibrilization mechanism of Aβ. Thus, we have conducted various Electron Paramagnetic Resonance (EPR) spectroscopy to elucidate the role of copper in the fibrilization mechanism of Aβ; we use multi-frequency, multi-technique pulsed EPR spectroscopy such as 34 GHz pulsed Electron Nuclear Double-Resonance (ENDOR), 9 GHz pulsed Electron Spin Echo Envelope Modulation (ESEEM) to determine the Cu^{II} ion coordination structure of CuAβ(1-40) in the processes of fibrilization of Aβ. Based on our recent EPR results, we will propose the fibrilization mechanism of CuAβ(1-40).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-223**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Application of RFQ/Cryo-Reduction EPR to Trap Intermediates of MMO

정한솔 홍수경[1] 이승재[2] 김선희[3,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 자연대학 화학나노과학과 [2]전북대학교 화학과 [3]한국기초과학지원연구원 서울서부센터

Methane Monooxygenase (MMO) is gaining attention due to its crucial role in global carbon cycle and to impede global warming by removing methane from the atmosphere. Moreover, the product of MMO's methane oxidation reaction, methanol, is also the source of alternative energy. To dates, the soluble form of MMO is known to have three protein components; (I) Hydroxylase (MMOH), (II) Reductase (MMOR), and (III) β-unit (MMOB). Due to the short life-time of intermediate species during oxidation, it is difficult to capture intermediates and the catalytic reaction cycle is not clarified yet. Thus, in order to elucidate the reaction mechanism, we utilized modified Rapid Freeze-Quench (RFQ) instrument. Rapid Freeze-Quench (RFQ) is a powerful tool to quench the intermediate and analyze the kinetics. After calculating total reaction time of the RFQ instrument, we are under studying the intermediate states of MMO during the oxidation reaction. Also, given the silent characteristics of di-ferric state in EPR, we performed cryo-reduction by γ- ray source at 77K to further trap the reaction intermediate. Consequently, our results, EPR studies coupled with RFQ an cryo-reduction, will provide an essential clue to comprehend the reaction mechanism of MMO.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-224**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Advanced EPR Characterization of Cu-Aβ-Inhibitor Ternary Complex

고유경 홍수경[1] 임미희[2] 김선희[3,*]

한국기초과학지원연구원 분석연구부 [1]이화여자대학교 자연대학 화학나노과학과 [2]UNIST 자연과학부/화학과 [3]한국기초과학지원연구원 서울서부센터

Alzheimer's disease (AD), a chronic neurodegenerative disease, has yielded severe societal problems and frustrated those patients' basic human rights. Notably, elevated concentrations of copper have been found in the brains of Alzheimer's patients. Therefore, it is deduced that copper ions play crucial roles in aggregation of Amyloid beta (Aβ) peptide. Meanwhile, recent studies on several organic inhibitors for Cu-Aβ aggregates suggest that the inhibitors are able to target and disassemble Cu-Aβ aggregation. Thus, clarification of the working mechanism of the inhibitors in Cu-Aβ system is essential. To illustrate the structure of Cu-Aβ-inhibitor ternary complexes and further elucidate the inhibition mechanism, multi-frequency and multi-technique Electron Paramagnetic Resonance (EPR) studies were conducted; 9 GHz Continuous Wave-EPR, 34 GHz pulsed Electron Nuclear Double Resonance (ENDOR), and 9 GHz pulsed Electron Spin Echo Envelope Modulation (ESEEM). Herein, we will present the novel structure of Cu-Aβ-inhibitor ternary complexes and the molecular working of inhibitors for Cu-Aβ. Furthermore, our recent result may provide a design rule of inhibitor molecules for Cu-Aβ aggregates, given advantages of EPR techniques in understanding the coordination of copper ions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-225**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Biomass Waste to Valuable Resource: Synthesis of Highly N-Doped Hierarchical Porous Carbon using Crab Shell for CO2 Adsorption and Supercapacitor Applications

김희수 김동관 유원철*

한양대학교 응용화학과

The fiber nature of the exoskeleton of Crab shell (CS) that consists of chitin-protein composites with CaCO3 and MgCO3 is converted to organic fibers, by which the CaCO3 and MgCO3 were removed using HCl treatment. Then these organic fibers were used to prepare Micro- Mesoporous carbon by carbonization, namely crab shell derived carbon nanofibers (CSCNs), and the subsequent CO2 activation process enables control of the porosity of the CSCNs. The activated porous carbon have a high specific surface area of 2430 m2 g-1 and a large pore volume of 1.21 cm3 g-1. As a CO2 adsorbent, the porous carbon has an outstanding CO2 adsorption capacity (6.09 mmol g-1 at 273K and 3.72 mmol g-1 at 298K under 1bar) and good CO2/N2 selectivity (33.6), which is decided from the single-component adsorption isotherms based on the ideal adsorption solution theory (IAST) method. In addition, as an electrode material, CSCN shows good electrical performance in 6M KOH aqueous electrolyte, with the specific capacitance of 220 F g-1 at a discharge current density of 1 A g-1 and prominent cycling stability for over 10000 cycles. This works shows a good instance for taking advantage of recycling food garbage and demonstrating applications in energy storage devices and gas sorbents.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-226**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

질소가 도핑 된 활성탄을 이용한 금속이온 흡착

김동관 김희수 유원철*

한양대학교 응용화학과

수질 속 미량 존재하는 Cu, Fe, Zn 등의 인체에 유해한 금속이온을 제거하기 위해 화학적 처리를 통하여 제거하는 경우 미량의 금속이온 제거가 어려울 뿐 아니라 화학약품을 사용해야 하는 번거로움이 있다. 이러한 경우 응집에 사용된 잔여 화학물질로 인한 오염 때문에 부작용 없이 효과적으로 수질 속의 금속이온을 제거 할 수 있는 흡착제의 개발이 필요하다. 이러한 이유로 인하여 수질 속 금속이온을 효율적으로 제거하기 위하여 고분자 전구체를 이용하여 활성탄을 제조하고, 활성화 과정을 통하여 기공특성 (표면적, 기공부피 등)을 조절하여 금속이온 흡착능과의 상관관계에 대한 연구를 진행하였다. 우선, Resorcinol - Formaldehyde 를 이용한 RF Polymer 를 합성한 후 탄화 과정을 진행하여 RF Carbon (RFC)을 제조했다. 이렇게 만들어진 탄소의 Porosity 증가에 따른 흡착능의 성능을 조사하기 위하여 CO2 활성화 과정 (C+CO2 -> 2CO 과정을 통하여 기공 발달) 을 진행하여 RFC 의 Porosity 를 향상시켰고 (RFC_CXX), 이렇게 활성화된 탄소들은 Porosity 가 증가함에 따라) 수질 속 금속 이온 흡착능이 상승하는 경향성을 나타냈다. 또한 물질의 Polarity 가 금속이온 흡착능에 미치는 영향을 조사하기위해 질소를 함유한 Dopamine 을 전구체로 이용하여, 질소가 도핑된 Melanin Carbon (MC) 을 제조하였다. CO2 활성화 과정을 이용하여 Porosity (표면적 and 기공부피)가 조절된 탄소를 제조 (MC_CXX) 하였으며 이렇게 만들어진 RFC 와 MC 활성탄의 금속이온 흡착능을 비교해 볼 때 질소가 도핑된 MC 활성탄의 금속 흡착능이 RFC 활성탄 보다 더 높은 것을 확인할 수 있다. 결론적으로 Porosity 가 증가 할수록 물리적인 흡착능의 증가로 인하여 수질 속 금속 이온의 제거 효율이 높아지며, 동일 Porosity 에서 N 의 함량이 많은, 즉 Polarity 가 높은 물질이 물리적인 흡착능 뿐만 아니라 금속이온과의 화학적인 흡착으로 인하여 더 높은 흡착능을 보여준다고 할 수 있다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-227**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Morphology-Preserved Transformation of MOFs to Metal/Metal Oxide Nanoparticles @ Carbon (M/MO@C) Composites and Electrochemical Applications

강민석 유원철*

한양대학교 응용화학과

Utilization of metal-organic frameworks (MOFs) as a precursor (or template) to synthesize metal or metal oxide via thermal treatments has been of great interest for heterogeneous catalysis and electrochemical applications. However, the morphology of produced metal or metal oxide is usually collapsed due to loss of organic moieties during heat treatments. Here, we report a facile method for morphology-preserved transformations of MOFs to metal/metal oxide@carbon (M/MO@C) composites. Catalytic-site specific polymerization occurs on the metal centers of MOFs via a gas-phase polymerization of phenol and formaldehyde (PF). The produced PF@MOF shows the same morphology and crystallinity as the MOF used. Upon careful choice of carbonization process, morphology-preserved M@C or MO@C composites can be synthesized. And their applications as anode materials for lithium ion batteries will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-228**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Pentane hydroconversion in Pt doped zeolites: Effect of frustrated lewis pairs in Pt doped zeolites under hydrogen pressures

조인화 최용남*

한국원자력연구원 중성자과학연구부

Normal pentane can be transformed in its shape or be cracked into smaller hydrocarbons by consuming reactive hydrogen ions, protons and hydrides. In this presentation, we show how a frustrated lewis pair formed in Pt doped zeolites affect the pentane hydroconversion process at various temperatures and hydrogen pressures. To study the effects, online GC, in situ x-ray diffraction, ex situ raman scattering measurements have been carried out and their results are presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-229**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

호스트-게스트 기반 약물전달용 다공성 실리카 나노입자의 제조

안준호 임나영 정종화*

경상대학교 화학과

속 빈 다공성 실리카 나노입자, 필러아렌이 도입된 금 나노입자 및 CdSe@SiO2 나노입자로 구성된 약물전달용 나노입자를 제조 하였다. 속 빈 다공성 실리카 나노입자는 산화철 나노입자에 CTAB(Cetrimonium bromide) 주형을 이용해 실리카 껍질층을 도입한 후 산처리를 통해 산화철 나노입자를 제거하여 제조 하였다. 필러아렌이 도입된 금 나노입자는 카복실기를 지니는 필러아렌과 금 나노입자 전구체 혼합용액에 NaBH4 를 첨가하여 제조 하였다. CdSe@SiO2 나노입자는 CdSe 나노입자 표면에 마이셀을 형성하여 실리카 전구물질을 도입하였다. 위의 세 종류의 나노입자는 각각 TEM, IR, Raman, UV-Vis 및 PL 분광기를 이용해 분석하였다. 또한 비결합성 상호작용을 이용해 실리카 나노입자를 중심으로 세 나노입자가 응집된 상태의 나노입자를 제조 하였으며, 이를 TEM, IR, Raman 분광기를 이용해 확인 하였다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-230**

발표분야: 무기화학

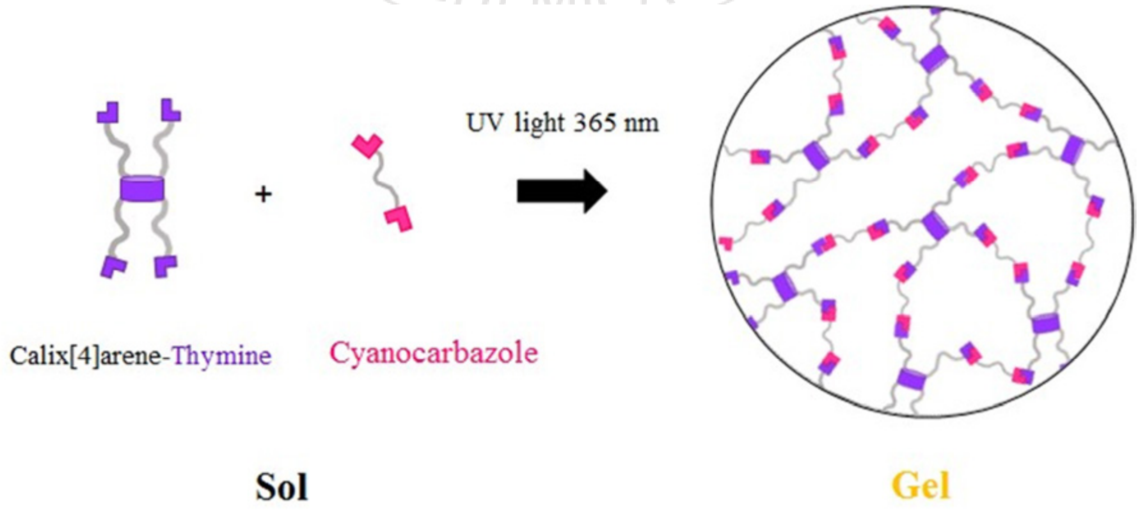
발표종류: 포스터, 발표일시: 목 11:00~12:30

칼릭스아렌 유도체와 시아노카바졸 유도체를 이용한 초분자 나노 구조체 합성

차유빈 최희경 정종화*

경상대학교 화학과

본 연구는 3-Cyanocarbazole 과 Thymine 기를 갖는 두 화합물의 수용액에 자외선 빛을 통해 공유결합을 형성하는 광가교결합을 통해 초분자 나노구조체를 개발하였다. 먼저 Thymine 이 도입된 Calix[4]arene 유도체를 3 단계, 알킬사슬의 양쪽에 3-Cyanocarbazole 을 도입한 빌딩블럭을 2 단계에 거쳐 합성하였다. 그리고 각각의 빌딩블럭을 혼합한 용매에 자외선을 조사하여 폴리머 반응을 통한 나노구조체 1 을 제조하여 NMR, SEM, UV, Light Scattering, IR 실험을 진행하였다. 따라서 본 학회에서는 자외선 조사에 의한 나노 구조체의 합성과 이에 따른 분광학적 특성에 대해 소개한다.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-231**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

칼릭스아렌 유도체가 도입된 AMP/Al-SiO$_2$ 나노입자의 세슘이온 흡착

임나영 안준호 박정수 정종화*

경상대학교 화학과

세슘 이온에 선택성을 갖는 ammonium molybdophosphate (AMP) 및 Calix[6]arene 유도체(L) 를 도입한 Aluminosilicate (L-AMP/Al-SiO$_2$) 를 제조하여 세슘이온에 대한 흡착특성을 분석하였다. 수열방법을 통해 젤상태의 Al-SiO$_2$ 을 제조한 후, CTAB/AMP 혼합 수용액을 첨가하여 수열반응을 진행하였다. 그 후 550℃에서 가열하고 산처리하여 유기물질과 불순물을 제거하였다. 아미드 결합을 통해 Calix[6]crown 유도체를 AMP/Al-SiO$_2$ 표면에 도입하였다. 제조된 L-AMP/Al-SiO$_2$ 는 IR 을 이용하여 작용기를 분석하였고, TGA 로 도입된 L 의 양을 측정하였다. XPS 로 Mo 가 있음을 확인했고, XRD 로 AMP 가 pore 내에 도입됨을 확인했다. 형광분광기를 이용한 선택성 실험결과 세슘 이온에 대해 선택적으로 turn-on 신호를 나타내었으며, 리간드의 약 500 배에 해당하는 세슘이온에 대한 감지가 가능함을 확인하였다. 또한 리간드가 도입된 효과로 세슘 이온에 대한 흡착성능이 향상되었음을 확인하였다. 리간드를 실리카 표면에 도입함으로써 AMP/Al-SiO$_2$ 나노입자의 세슘 이온에 대한 흡착율이 향상되었음을 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-232**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Chirality control of hydrogel by transition metal ions

최희경 서효원 정종화*

경상대학교 화학과

Bipyridine-based precursor **1** containing chiral D-alanine and precursor **2** containing achiral glyclyglycine were designed and synthesized. Each of the precursor **1** and **2** is a sol state in aqueous media, in contrast, the mixture of **1** and **2** could form a hydrogel possessing a left-handed helicity by co-assembly. The helicity of the hydrogel could controlled by addition of Ni^{2+} ions. A right-handed helical assembly was confirmed by a positive CD signal at 324 nm in the case of the hydrogel with 0.1-0.5 equiv. of Ni^{2+}, indicating inversion of the chirality of the surrounding molecular environment. Interestingly, the CD signal was returned to negative area with more than 0.6 equiv. of Ni^{2+}. This result is attributed to the conversion of six coordinated Ni^{2+} exhibiting red color into four coordinated form exhibiting blue color by increase of Ni^{2+}.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-233**

발표분야: 무기화학

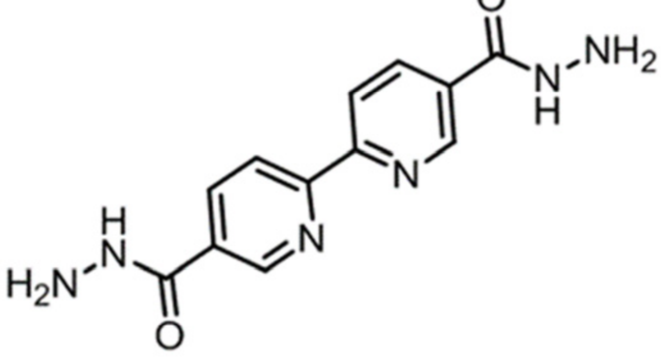
발표종류: 포스터, 발표일시: 목 11:00~12:30

용매교환을 통한 카이랄성 하이드로젤 제조

고미선 최희경 정종화*

경상대학교 화학과

본 연구에서는 히드라진기를 갖는 피리딘 유도체 **1** 을 합성하였고, 하이드라존 반응을 통해 고분자성 젤을 제조하였다. 하이드라존 반응에 의해서 제조된 고분자성 젤을 물에 18 시간 동안 담궈두는 방법으로 하이드로젤을 제조하였다.제조된 하이드로젤의 나선특성을 원편광 이색성 분광기를 이용하여 측정해본 결과 젤은 나선성을 그대로 유지하고 있었다. 또한 적외선 분광법, 2 차원 면적 검출 X 선 분광기를 통하여 하이드로젤의 구조변환을 규명하였고, 현미경을 통하여 모폴로지의 변화를 관찰하였다. 섬유형태를 갖던 고분자젤의 모폴로지는 용매교환 후 벌집형태로 변화하였다. 반면 유동계를 이용하여 하이드로젤의 점탄성이 크게 증가하는 것 또한 확인하였다. 본 심포지움에서는 용매교환을 통해 제조된 하이드로젤의 특성에 대하여 소개하고자 한다.



1

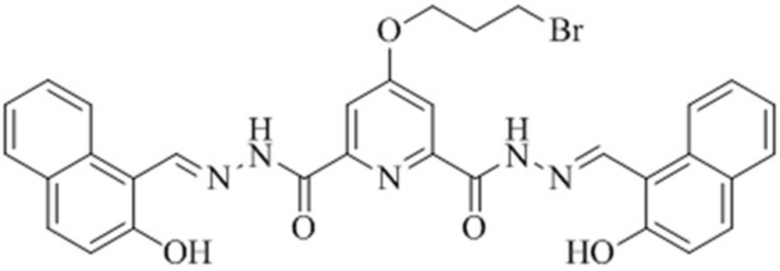
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-234**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Naphthalene-based organic-inorganic hybrid fluorescent sensor for detection of Cs^+

박정수 최연원 정종화*

경상대학교 화학과

The naphthalene-based ligand **1** has been synthesized by multi-steps. The fluorescence properties of **1** upon addition various metal ions were observed by using fluorescence spectrophotometer. As the result, interestingly, **1** was found to display dramatically enhanced fluorescence quenching effect upon addition of Cs^+, but not with any other metal ions such as Li^+, Na^+, K^+, Rb^+, Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Zn^{2+} and Ni^{2+}. The binding between **1** and Cs^+ led to a 1:1 stoichiometric ratio by Job plot. Furthermore, we expect that NP-**1** can act as an adsorbent for Cs^+. NP-**1** effectively adsorbed Cs^+ in aqueous solution. These results indicate that NP-**1** is useful as an adsorbent to remove Cs^+.



1

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-235**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fluorescence imaging for Fe^{3+} in *Arabidopsis* by using simple naphthalene-based ligands

문규리 최희경 서효원 정종화*

경상대학교 화학과

A main source of Fe^{3+} exposure for mammals is through plants consumption. Thus, sensitive and selective Fe^{3+} detection in plants tissue is a significant and an urgent need. Although fluorescence probes have been reported for Fe^{3+} in water, the detection of endogenous biological Fe^{3+} in plants tissue remains to be refined due to the high background signal and the thickness of the plant tissue that can hamper an effective application of traditional one-photon excitation. To address these issues, we have synthesized naphthalene-based probes, **1** and **1A**. Upon an addition of Fe^{3+} in water-methanol (1:1, v/v, pH 7), the fluorescence probes of **1** and **1A** were found to dramatically decrease, but no other metal ions had this effect. More interestingly, **1A**, which had no diethyl 2,2′-(phenylazanediyl)diacetate moiety, also exhibited high selectivity for Fe^{3+}. These results clearly indicate that the Fe^{3+} was bound to the nitrogen and oxygen atoms located near the naphthalene moiety. Furthermore, chemical probes of **1** and **1A** were embedded into nanofibrous membrane films NF-**1** and NF-**1A**, respectively, prepared by the electrospinning method for use as a portable chemical probe. Fluorescence changes were examined by immersing the films into solution of various metal ions. The strong fluorescence intensity of both NF-**1** and NF-**1A** dramatically decreased in accordance with concentration of Fe^{3+} onto the film, which was a "turn-off" system. In contrast, no significant changes of fluorescence intensity were observed compared that of other metal ions, such as Na^+, K^+, Zn^{2+}, Pb^{2+}, Mn^{2+}, Cu^{2+}, Co^{2+}, Ca^{2+}, Fe^{2+}, and Cd^{2+}. The results indicate that both NF-**1** and NF-**1A** could be used to selectively detect Fe^{3+}. We also investigated the practicality of both **1** and **1A** as imaging probes for Fe^{3+} to operate within living systems like plants. Chemical probes of both **1** and **1A** were tested for fluorescence imaging of Fe^{3+} in Arabidopsis. As expected, the fluorescence probes displayed high fluorescence imaging for Fe^{3+} in *Arabidopsis*.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-236**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Control of Cyanosilbene-Based Self-Assembeld Nanostructure as Mirochondria Imaging Probe

김가영 정종화*

경상대학교 화학과

Subcellular organelle-specific reagents for simultaneous tumor targeting, imaging, and treatment are of enormous interest in cancer therapy. Herein, we describe the design and synthesis of mitochondria-targeting nanostructure unit composed of a lipophilic triphenylphosphonium cation (TPP) for efficient mitochondrial targeting and a cyanostilbene fluorophore for fluorescence-based real-time tracking of its uptake and distribution into various subcellular compartments which can undergo aggregation-induced emission (AIE). Owing to the more negative mitochondrial membrane potential of cancer cells than normal cells, the probe **1** can selectively accumulate in cancer-cell mitochondria and light up its fluorescence. More importantly, the probe exhibits selective cytotoxicity for studied cancer cells over normal cells. The high potency of **1** correlates with its strong ability to aggregate in mitochondria, which can efficiently decrease the mitochondria membrane potential and increase the level of intracellular reactive oxygen species (ROS) in cancer cells. The mitochondrial light-up probe provides a unique strategy for potential image-guided therapy of cancer cells.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-237**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Terpyridine-Based Chiral Supermolecular Metallogels with Lanthanide and Their Applications

김채린 김가영 정종화*

경상대학교 화학과

Lanthanide ion-based supramolecular hydrogels have drawn considerable attention, due to their broad applications such as their unique redox, optical, electronic, and magnetic properties in chemistry, materials, and biological sciences. In particular, lanthanide ion-based gels are specific interest as they show narrow band emission with high quantum yields and different colors. Here we present the helical luminescent supramolecular hydrogels with Tb(III) and Eu(III) and their inkjet printing pattering in application. The luminescent gels, which exhibit three color emissions such as red, green, and blue could be prepared with Eu(III) and Tb(III). These gels showed well-defined right-handed helical nanofiber by coordination bond by AFM observations. In particular, the coordination bond in supramolecular hydrogels was strongly influenced in rheological properties. The time-resolved luminescence life times of gel-Tb and gel-Eu enhanced ~50000-100000 folds in compared to gel-1. More interestingly, we also developed a water-compatible the inkjet printing system that can be employed to generate luminescent supramolecular gels on the paper, which resulted in red, green, and blue emissions.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

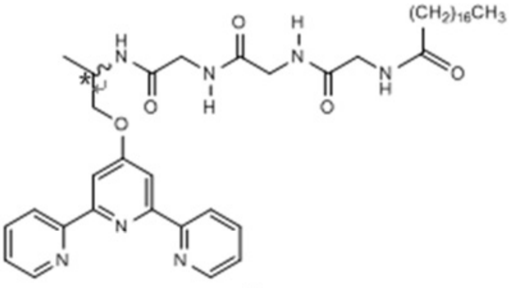
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-238**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

코발트 금속 이온의 당량에 따른 초분자 나선 구조 제어

박혜송 김가영 정종화*

경상대학교 화학과

.본 연구는 터피리딘 유도체와 코발트 금속 이온이 배위 고분자를 형성할 때, 코발트 금속 이온의 당량에 따라 발생하는 초분자의 구조 변환에 대한 연구이다. 코발트와 배위 가능한 터피리딘과 카이랄 성을 지닌 2-amino-1-propanol 과 초분자 젤 형성을 위한 peptide 구조를 가진 긴 사슬을 도입한 화합물 1 를 합성하여 NMR, MS 을 통해 구조를 확인하였다. 터피리딘 유도체(1)는 THF 용매 조건 하에서 코발트 금속 이온이 0.0 당량에서 3.0 당량 존재할 때 초분자 젤이 제조되었다. 이 코발트 착물은 CD 와 UV 을 통해 당량 에 따른 흡수와 CD intensity 가 관찰되었고, 특정 당량에서 카이랄 반전이 일어나는 것을 확인하였다. 또한 이 착물을 ESI-Mass 로 일부 당량에서 측정하여 이를 토대로 각 당량에서 초분자의 배위 구조를 예측하였다.



1

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-239**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

MOF-derived Cu@C Composite as high efficient catalyst for various organic reactions

김보람 김혜련 김명진[1] 김진호[1,*] 이창연[2,*]

인천대학교 에너지화학공학과 [1]인천대학교 화학과 [2]인천대학교 에너지 화학공학과

Metal-organic frameworks (MOFs) have attracted great interest due to their high specific surface area, pore volume and the large density of active sites. Therefore, MOFs are ideal candidates for heterogeneous catalyst. However, MOFs system have poor reusability and stability because of the relatively weak coordination bond between the metal and the organic linker in MOFs. Here in, we synthesize Cu@C catalyst, which is generated by simple pyrolysis of Cu3(BTC)2. A developed Cu@C catalyst exhibit outstanding performance for aerobic oxidation of alcohols, aerobic oxidative conversions of benzaldehydes into benzonitriles and three-component coupling reaction of terminal alkyne, sulfonyl azide and amine. Furthermore, Cu@C system reveal broad scope for the substrate and is usable without the loss of catalytic activity.This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2016R1A2B4010376)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-240**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dual-functional electrocatalyst derived from porphyrin-embedded metal-organic frameworks (MOFs)

정유일 박경철 GUPTA GAJENDRA[1] 이창연[1,*]

인천대학교 에너지화학공학과 [1]인천대학교 에너지 화학공학과

본 발표는 메탈 이온과 유기 리간드가 배위결합하여 만들어지는 금속-유기 골격체(Metal-Organic Frameworks (MOFs))를 활용하여 비백금계 Oxygen Reduction reaction (ORR)과 Hydrogen evolution reaction (HER)을 위한 촉매제조 및 활성에 관한 연구내용의 발표이다. 금속 유기 골격체는 다공성 물질로 표면적과 기공 부피가 크고 화학적 특성을 조절 할 수 있다는 장점을 지니고 있다. 이러한 장점을 이용해 내부 기공이 큰 금속-유기 골격체에 Iron-porphyrin (Fe-TCPP)를 담지하고 열분해를 통해 Fe-N-C (Iron-Nitrogen-Carbon)의 촉매 활성점을 가지는 ORR, HER Dual-functional electrocatalyst 를 합성하였다. 합성된 촉매는 BET, XRD, XPS, TEM, EDS 등의 분석을 통해 특성을 파악하였고, CV, RDE Polarization Curve, K-L plot 을 통해 ORR 촉매로서의 성능을 측정하였고, Impedence, CV, Tafel plot, Polarization Curve, Stability test 를 통해 HER 촉매로서의 성능을 측정하였다.Acknowledgement : This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2013R1A1A1058839).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-241**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Ammonia from a Molybdenum Nitrido Complex

배대영 이은성*

POSTECH 화학과

Transition metal nitrido complexes have attracted interest due to their similarity of a potential intermediate of catalytic reaction pathway of the nitrogenase and capability of dinitrogen reduction to ammonia in a catalytic way or conversion to nitrogen containing molecules. Even though many researches have been proceeding to find out catalytic reactivities of transition metal nitrido complexes with various ligands, metal nitrido complexes binding oxygen ligands have been less studied. Herein, we report a new type of molybdenum nitrido complex binding with tetradentate triphenolate amine and tert-butoxide ligand and its quantitative ammonia formation in the presence of protons and electrons under mild conditions. Based on electronic and structural properties of the nitrido complex, it is expected that the complex will have catalytic ability toward dinitrogen conversion to ammonia.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-242**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Hydrolytic Conversion of Preceramic Polymers into Silicate Glass Coatings

황윤호 김동표*

POSTECH 화학공학과

In this study, two types of preceramic polymers were used to form silicate glass coatings with different wettability via hydrolysis either under harsh or mild conditions. Allylhydridopolycarbosilane (AHPCS) and polyvinylsilazane (PVSZ) were spin-coated on Si substrate and consolidated by photo- and thermal-curing and subjected to hydrolysis for conversion to the silicate glass phase. The contact angle of the both hydrophobic cured polymers decreased from 91o–92o to 18o–36o with little difference, when hydrolyzed in strong alkaline of NaOH solution at room temperature. However, soft hydrolysis in ammonia vapor at 80oC showed that the AHPCS derived silicate surface showed the moderate contact angle 63o, while the PVSZ derived silicate became very hydrophobic surface with the contact angle 101o presumably due to re-oriented alkyl groups. Eventually, it was demonstrated that the surface wettability of the hydrolyzed silicates was controlled with the polymer chemistry and the hydrolytic conditions upon the preceramic polymer-to-silica conversion.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-243**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An *N*-Heterocyclic Carbene Stabilized SF_2 Complex and Its Dimer Form

임수빈 이은성*

POSTECH 화학과

Analogous to hypervalent iodine compounds, which enable to transfer electrophilic groups such as trifluoromethyl, aryl, amine, halogen and other groups to substrates,[1] the Alcarazo group reported synthesis of imidazolium sulfuranes containing hypervalent sulfur with bromine, chloride or cyanide group. The cyanide group was further transferred to other molecules by C-H bond activation.[2] Inspired by the work, we synthesized imidazolium sulfuranes containing hypervalent sulfur with fluorine utilized by *N*-heterocyclic carbenes (NHCs) and xenon difluoride. The imidazolium diflurosulfuranes were characterized by NMR spectroscopy and X-ray crystallography. Their fluorine atom transfer reactivity includes fluorination of benzoic acid to afford corresponding benzoyl fluoride. Although the fluorination reactivity of the imidazolium diflurosulfuranes is very limited unlike other deoxyfluorinating sulfur-based reagents, synthetic methods and structural characterization of NHC-SF_2 including an interesting sulfurane fluoride dimer will adds another important example of carbenes' unique reactivity.Reference(1) Merritt, E.; Olofsson, B. Angew. Chem., Int. Ed. 2009, 48, 9052−9070.(2) Talavera, G.; Peña, J.; Alcarazo, M. J. Am. Chem. Soc. 2015, 137, 8704−8707.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-244**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthetic Control of Coincidental Formation of N-Heterocyclic Carbene-Copper(I) Complex within 2D and 3D Metal-organic Frameworks

이현정 권현철[1] 김자헌[2] 김기문 이은성*

POSTECH 화학과 [1]POSTECH 화학화 [2]숭실대학교 화학과

Two-dimensional (2D) copper paddle-wheel based metal-organic frameworks containing an imidazolium unit or an N-heterocyclic carbene copper(I) complex have been successfully prepared and characterized by X-ray crystallography. The two 2D MOFs are almost identical except the environment of N-heterocyclic carbene center, which differs from the formation of N-heterocyclic carbene-copper(I) complex in the 2D MOF. Higher concentration of the copper source allowed 3D metal-organic framework with completely different copper connectivity. The choice of copper metal sources under different solvent systems allows such different coordination environment at the carbene center. Furthermore, borylation of aryl bromides proves that the MOF containing the NHC-copper chloride complex is the active catalyst, demonstrating that the copper(II) ions in the paddle wheel structure does not catalyze the borylation reaction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-245**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Transition Metal Coordination Chemistry of Hexa(2-pyridyl)benzene

권현철 이은성*

POSTECH 화학과

Multi-metallic or metal cluster system have been of great interests due to their potential applications in catalysis because multi-metallic or cluster systems have been found to lower activation energy of catalytic reactions involving redox chemistry via cooperative or synergistic effects. To envision such systems, we have synthesized a hexa(2-pyridyl)benzene ligand, which contains six pyridyl units to assist transition metal coordination in a multi-metallic mode. The ligand was thus applied for complexation with a variety of transition metals such as copper, silver, nickel, palladium, etc. Full-characterization of those complexes will presented including X-ray structural analysis. In addition, redox chemistry and catalytic activities in multi-palladium system will be added in the poster presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-246**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ferric Ion Accumulation in the Walls of Metabollically Dormant Saccharomyces cerevisiae Cells as Another Form of Iron Storage

박진규* **Paul A. Lindahl**[1]

한국원자력연구원 원자력화학연구부 [1]Texas A&M University, U.S.A.

Iron (Fe) is an essential element for cellular metabolism playing numerous roles in enzyme catalysis, electron transfer processes, and small-molecule binding and activation, etc. On the other hand, Fe can also be detrimental to the cell, because certain forms participate in Fenton chemistry generating reactive oxygen species (ROS) which can thus damage DNA, proteins, and membranes. Hence, the trafficking and regulation of Fe are remarkably important in cellular metabolism. Mitochondria, Golgi apparatus and endoplasmic reticulum are known to be crucial Fe regulatory organelles and vacuoles are major storage for intracellular Fe. In this study, Fe in Saccharomyces cerevisiae cell was monitored by biophysical and bioanalytical tools such as Mossbauer and electron paramagnetic resonance spectroscopy and inductively-coupled plasma mass spectrometry, while the cells were grown to metabolically dormant status. It turned out that the cells accumulate Fe in the cell walls mainly in the form of mononuclear nonheme high-spin Fe (III). When the dormant cells were incubated in a fresh but Fe-deficient medium, cells were able to grow using the accumulated Fe, indicating that the cell walls might function as an Fe storage. More details will be discussed in the presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-247**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A new Zr-based metal-organic framework with mixed heterolinker ligands

김혜현 원소미 나명수*

UNIST 화학과

The preparation of metal-organic frameworks(MOFs) that contain mixed heterolinker ligands is important for the modulation and the tune of the framework properties. Despite tremendous endeavor, it is still difficult to synthesize a new Zr-based MOF with mixed heterolinker ligands. Recently, preparations of a series of new Zr-MOFs of 10-, 11- and 12-connectivity that contain mixed heterolinker ligands are reported via sequential insertions of additional linkers into a 8-c Zr-MOF. However, one step preparation of a Zr-MOF with mixed heterolinker ligands is yet to be reported. Here, we report the one-pot solvothermal preparation of a new Zr-MOF with mixed heterolinker ligands of different lengths. The reaction of $ZrOCl_2$ with both fumaric acid(H_2fum) and 2,6-naphthalene dicarboxylic acid(H_2ndc) led either a mixture of two different MOFs, MOF-801 and DUT-52, containing each single ligand or a pure single phase of a stoichiometric mixed ligand ratio depending on the ratio of the mixed ligands in the reaction conditions. The structure of the new Zr-MOF that contain both fum and ndc in a stoichiometric 1:1 ratio, $[Zr_6O_4(OH)_4(fum)_3(ndc)_3]$ (ZFN-1), was solved using X-ray powder diffraction. Even though ZFN-1 contains two different lengths of ligands, it is a net of a 12-c fcu topology. The Zr6 clusters in the frameworks are interconnected via fum to form a 2-D sheet of 6-c hxl topology and the 2-D sheets are further interconnected by using ndc to form a net of 12-c fcu topology. ZFN-1 showed the reduced stability than that of the corresponding isoreticular Zr-MOF of either pure fum or ndc probably due to the structural strain caused by the two different length of the heterolinker ligands.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-248**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Reversible Single-Crystal-to-Single-Crystal Transformations of MOFs via Postsynthetic Exchange, Deletion and Insertion of Ligands that Accompany Two-dimensional Reorganizations of Framework Structures

신선영 정석 한승완 나명수*

UNIST 화학과

A three-periodic (3-P) metal-organic framework (MOF) based on a one-periodic (1-P) rhomboidal chain as a supermolecular building block (SBB) can be transformed to another stable 3-P MOF via postsynthetic exchange of ligands in single-crystal-to-single-crystal (SCSC) fashion that accompanies the unprecedented two-dimensional (2-D) structural reorganization. The enhanced framework rigidity of the new MOF allows partial but systematic deletion of some organic linkers from the framework, which leads to the other 3-P MOF. The SCSC transformations can occur reversibly by postsynthetic exchange, deletion, and insertion of the ligands, where the stable 1-P SBB plays a pivotal role during the transformations that accompany significant 2-D reorganization of the framework structures.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-249**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced Hydrogen Photoproduction with a Pyrene-pendant Metal Catalysts on Reduced Graphene Oxide

김진홍* 김수진 장하윤[1] 이주현[2] 박유미[3] 전유정[2]

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학.나노과학과 [2]이화여자대학교 화학나노과학과 [3]이화여자대학교 화학나노과학

Reduced graphene oxide (rGO), which is highly dispersed in water due to its hydrophilic oxygen functional groups is intensively utilized to prepare efficient systems for optical sensors, catalysts, light antennas, and other applications. Noncovalent • ;• •stacking interactions of various molecules for the modification of conjugated carbon nanomaterials, such as carbon nanotubes and graphene, have been used to immobilize chemical/biological probes and catalysts. Examples using carbon nanomaterials immobilized with molecular metal catalysts, especially in photocatalytic reactions requiring a wide range of light absorption and an excellent electron transfer process, are relatively rare. The conversion of formic acid/formate in the presence of homogeneous metal catalysts has also been studied for the production of hydrogen. Many catalytic systems using molecular metal complexes have used thermal energy in order to achieve high conversion rates and yields. We present the visible light-driven photoproduction of hydrogen using a pyrene-derivatized rhodium complex anchored on rGO by • •• •stacking interactions. First, we show a surprising enhancement effect of rGO on hydrogen photoproduction with the molecular rhodium catalyst and formate in the presence of PtNPs upon visible light irradiation in an aqueous solution. In addition, the pyrene-pedant Ni catalyst immobilized on rGO shows enhanced photocatalytic hydrogen production.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-250**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An Emission Probe Specific for Cr3+ and Cu2+: Solvent-dependence

김진홍[*] 장하윤[1] 박유미[2] 이주현[3] 전유정[3]

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학.나노과학과 [2]이화여자대학교 화학나노과학 [3]이화여자대학교 화학나노과학과

A new chemosensor containing julolidine-naphthylamine was prepared for sensing specific metal ions. Probe EW1 afforded a broad low fluorescence at 500-600 nm in acetonitrile, but gave a relatively stronger fluorescence at 540 nm in methanol. This chemosensor showed a selective turn-on emission for Cr3+ in CH3CN. Upon treatment with Cr3+, a strong emission was observed at 515 nm, but other metal ions, such as K+, Ag+, Ca2+, Zn2+, Co2+, Ni2+, Cu2+, Cd2+, Hg2+, Fe2+, Fe3+, failed to induce such an emission band. A clean isosbestic point appeared at 405 nm in the UV-vis titration with Cr3+. The emission intensity of the chemosensor was enhanced with incremental addition of Cr3+, indicating the formation of a 1:1 complex of the probe EW1 and chromium ion. However, this probe showed a selective turn-off response with Cu2+ in CH3OH. The emission band of the chemosensor at 540 nm was quenched only with Cu2+ and not with other control metal ions. The absorption band of the chemosensor at 410 nm progressively decreased, and a new absorption at 390 nm appeared upon progressive addition of Cu2+. All spectroscopic titration experiments and ESI mass data provided evidence for the formation of a 1:1 complex between the chemosensor and Cu2+.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-251**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Stepwise Chemical Activation of Open-Metal Sites in Copper-Based Metal-Organic Framework HKUST-1

배진희 정낙천[1,*]

DGIST 신물질과학전공 [1]DGIST 신물질과학과

Metal-organic frameworks (MOFs) are an intriguing class of nanoporous materials that can be readily self-assembled by combining metal ions and organic ligands. With the extended nano-porosity and large internal surface area, MOFs have been examined as candidates for applications. In particular, the open coordination site(OCS) on nodal metal ion has shown considerable potential in its role for the applications in i.e., high ion transport and efficient gas sorption. Thus, the activation of MOFs• the removal of pre-coordinated solvent molecules (typically used in during the synthesis) from the OCSs• has been thought as a prerequisite step for those applications. The thermal activation (TA), which is normally performed by applying heat and vacuum, has been a unique way to remove the OCS-coordinated solvent molecule, whereas the other four methods are only useful for removing pore-filling solvents. Given that the high temperature can lead to structural damage to MOFs, low-temperature process will be conceivably a promising way for OCS activation, compared to the cumbersome, pricey heat-and-vacuum technique.Recently, we have discovered a new, chemical method to activate the OCS, namely “chemical activation” (CA). This process is performed just by soaking MOF samples into dichloromethane (DCM) for several minutes at room temperature. Although this CA method is quite useful for low-temperature activation, strongly coordinated solvent such as DMF and DMSO cannot be adaptable to this CA method because they are not readily replaced by DCM whose coordination is very weak. In this poster, we present an advanced CA method, “multistep chemical activation”. With this strategy, we could completely remove the DMF solvent coordinated to the OCS sites in HKUST-1 without structural damage.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-252**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Facile Route to Fabrication of HKUST-1 Film on Copper Substrate

지훈 정낙천[1,*]

DGIST 신물질과학전공 [1]DGIST 신물질과학과

Metal-organic frameworks (MOFs) are an interesting class of nanoporous crystalline solids that can be readily self-assembled by combining metal ions (or clusters) and multitopic organic ligands via coordination bondings. Often characterized by well-defined nano-porosity and large internal surface area, MOFs are being examined as candidates for applications in chemical separations, gas storage, ionic conduction, and chemical sensing. In particular, electronic or ionic conductive MOF materials have shown considerable potential for their conceivable applications in i.e., electrical and electrochemical devices. But, such applications are typically based on the platform of films. Thus, the fabrication of MOF films has been thought as an essential step prior to the applications. To date, several methods for synthesizing MOF film have been suggested• surface modification and subsequent primary (or direct) growth, spin-coating, electrochemical deposition, alternating Layer-by-Layer (LBL) growth, and Langmuir-Blodgett deposition. These fabrication methods are often combined with the chemical functionalization of substrate surface in order to enhance the adhesive force in the junction between MOF film and metal substrate and thereby, synthesize chemically robust MOF film on the metal. However, it has proven difficult to enhance the adhesive force because the covalent bond formed by the functionalization is not strong as well enough to bind the film, or the adhesion force is weak physical interaction unless the substrate is not functionalized. In addition to this, the film will be substantially robust if MOF crystal domains are crossly interconnected. Due to the lack of strong adhesive force and chemical link between domains, however, MOF films are often peel off from the metal substrates. Thus, the synthesis of robust MOF films can be feasible when these two factors are considered. In this poster, we present a successful method to synthesize robust HKUST-1 films on metallic Cu substrate. The fabrication could be achieved by soaking Cu substrate into a prepared solution only for 5 min. Further, we demonstrate that this method is highly useful for fabricating patterned MOF films.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-253**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Synthesis of ZnO Nanorods with Different Aspect Ratios and Their Optical Properties

ruqia bibi 최상일[1,*]

경북대학교 자연과학대학 화학과 [1]경북대학교 화학과

One-dimensional (1-D) ZnO nanorods with different aspect ratios (length to diameter) were prepared by a direct solvothermal method using octanol as a solvent. We investigated the concentration effect of Zn precursor for the manipulation of aspect ratio of ZnO nanorods. Morphological and structural characterizations were carried out by X-ray diffraction and transmission electron microscopy. As-obtained ZnO nanorods were determined to be a single crystalline nature with their c-axis as the primary growth direction. UV-Vis and photoluminescence spectra of ZnO nanorods exhibited a red-shift of UV absorption from 347 to 356 nm and a blue-shift of UV emission from 393 to 388 nm, respectively. A good crystallinity of ZnO nanorods was demonstrated with a strong UV emission together with a weak and broad green emission band from 528 to 552 nm, which is typically attributed to the oxygen defects.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-254**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Experimental and computational studies of formicacid dehydrogenation over PdAu: influence ofensemble and ligand effects on catalysis

최수빈 박현서[1,*] 윤창원[1,*]

경희대학교 KHU-KIST 융합과학기술학과 [1]한국과학기술연구원(KIST) 연료전지연구센터

We elucidated the potential role of the ligand and ensemble effects in improving formic acid (FA) dehydrogenation over PdAu catalysts by employing both experimental and theoretical studies. Relevant energetics associated with FA decomposition were considered by preparing PdAu model catalysts with four distinct surface atomic arrangements. Among these PdAu surfaces, the Pd3Au1 surface was found to have the lowest reaction pathway and kinetic barrier for FA dehydrogenation, implying that the Pd trimer played an important role in stabilizing intermediates. Consistent with the theoretical results, the experimentally modified PdAu catalysts showed different FA dehydrogenation activities depending on the surface arrangements. In addition, the electronic interaction between the surface and subsurface layers further proved to contribute to the increased activity of PdAu catalysts via modification of Pd d states.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-255**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Phenyl-Vinyl-Based Polysiloxane Electrolytes by Using Oligohydrosiloxanes

정대윤 손홍래*

조선대학교 화학과

For the synthesis of phenyl-vinyl-based polysiloxane electrolytes, novel cross-linking agents containing siliconhydride such as linear hydrosiloxane oligomers have been discovered via hydrosilylation reaction. Phenyl-vinyl-based oligosiloxanes were synthesized from the reaction of diphenylsilanediol and vinyltrimethoxysilane through a nonhydrolytic sol-gel condensation. linear hydrosiloxane oligomers containing Si-H moiety were obtained from the reaction of dichlorodimethylsilane and dichlorophenylsilane. Dimethylchlorosilane was used as a ending group for the linear hydrosiloxane oligomers. The reaction of phenyl-vinyl-based oligosiloxanes and linear hydrosiloxane oligomers in the present of Pt catalyst was carried out for the synthesis of polysiloxane electrolytes. The prepared phenyl-vinylbased polysiloxane electrolytes showed a good refractive index, high hardness, and great transmittance. The comparison to previously known phenyltris(dimethylsiloxy)silane as a cross-linking agent has been reported. This research was financially supported by the Ministry of Trade, Industry, and Energy (MOTIE), Korea, under the “Regional Specialized Industry Development Program” supervised by the Korea Institute for Advancement of Technology (KIAT).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-256**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Phenylvinyl Polysiloxane Electrolytes with Various Phenyl Derivatives

정대윤 손홍래*

조선대학교 화학과

Phenylvinyl polysiloxane (PVPS) electrolytes with various phenyl derivatives has been successfully achieved. The phenyl derivatives used in phenylvinyl polysiloxane electrolytes are phenyl and mesityl group. Thermally stable transparent PVPS electrolytes with high refractive index was synthesized by the thermal curing reaction of phenylvinyl oligosiloxanes (PVOS). PVOS was obtained by a sol-gel condensation process between vinyltrimethoxysilane (VTMS) and diphenylsilanediol (DPSD). We have investigated the effect of phenyl derivatives on PVOS electrolytes. Instead of using DPSD, dimestylsilanediol (DMSD) was used for the synthesis of mesitylvinyl oligosiloxane (MVOS). DMSD was synthesized from the reaction of 2 equivalents of mesityllithium and silicon tetrachloride. To obtain mesitylvinyl polysiloxane (MVPS) electrolytes, MVOS was thermally cured at 150 ℃ for 3 hours. The comparison with DPSD was achieved. The physical properties such as an optical transmittance, refractive index, and harness were measured. This research was financially supported by the Ministry of Trade, Industry, and Energy (MOTIE), Korea, under the “Regional Specialized Industry Development Program” supervised by the Korea Institute for Advancement of Technology (KIAT).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-257**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Phenyl-Vinyl-Based Polysiloxane/Metal Oxide Nanoparticle Hybrimer

정대윤 조승주[1,*] 손홍래[*]

조선대학교 화학과 [1]조선대학교 의학과

Phenyl-vinyl-based polysiloxane (PVPS)/metal oxide nanoparticles (MONPs) hybrimer was synthesized from the reaction of PVPS and MONPs via hydrosilylation in the presence of platinum catalyst. MONPs were surface-derivatized from the reaction of MONPs with dimethylchlorosilane to give SiH-terminated MONPs. Si-H moiety of the MONPs was used for a covalent attachment with vinyl group of PVPS via hydrosilylation. The physical properties such as an optical transmittance, refractive index, and harness of PVPS/ MONPs hybrimer were investigated with various curing times and precursor compositions. Optical characterizations of MONPs were achieved by using UV-Vis and photoluminescence spectroscopy. To tune the refractive index of PVPS/ MONPs hybrimer, thermal stability was investigated upon baking. This research was financially supported by the Ministry of Trade, Industry, and Energy (MOTIE), Korea, under the “Regional Specialized Industry Development Program” supervised by the Korea Institute for Advancement of Technology (KIAT).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-258**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ultra-Fast Curing of Epoxy-Based Polysiloxane Electrolytes Showing High Refractive and Transparent Optical Properties

조보민 손홍래*

조선대학교 화학과

The epoxy-based oligosiloxanes were synthesized from the reaction of 3-glycidoxypropyltrimethoxysilane, diphenylsilanediol (DPSD). Previously known cross-linking agent such as a methyl hexa-hydrophthalic anhydride (MHHPA) for the synthesis of epoxy-based polysiloxane electrolytes in the present of amine catalyst showed disadvantage in terms of long curing time. To obtain suitable hardness for polysiloxane electrolytes, the curing time to complete the reaction requires 12 hours. Here, we reported new aromatic anhydrides as a ultra-fast curing agent for the synthesis of epoxy-based polysiloxane electrolytes. The curing process with non-aromatic anhydride requires usually more than 12 hours. However the curing process with aromatic anhydrides requires only about 30 min to obtain a suitable hardness. Prepared epoxy-based polysiloxane electrolytes exhibited an ultra-fast curing time, good refractive index, and high hardness and transmittance.This research was financially supported by the Ministry of Trade, Industry, and Energy (MOTIE), Korea, under the “Regional Specialized Industry Development Program” supervised by the Korea Institute for Advancement of Technology (KIAT).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-259**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

High Refractive Polysiloxane Hybrimer Based on Dendrimer-Type Siloxane

조보민 손홍래*

조선대학교 화학과

Phenyl-vinyl-oligosiloxane (PVO) has been was synthesized by nonhydrolytic sol-gel condensation process from the reaction of vinyltrimethoxysilane (VTMS) and diphenylsilanediol (DPSD). Barium hydroxide monohydrate was used as a catalyst and promotes the direct condensation reaction between the methoxy radical of VTMS and diol radical of DPSD from siloxane bonds. The 1,3,5-tris(dimethylhydrosilyl)benzene (TDMSB), crosslinking agent, was synthesized through in situ Grignard reactions of 1,3,5-tribromobenzene with chlorodimethylsilane. The synthesized PVO were thermal cured with a cross-linker, TDMSB, through a hydrosilylation reaction under a Pt catalyst, Platinum cyclovinylmethyl-siloxane complex (Pt0 . [CH2=Ch(Me)SiO]4). This research was financially supported by the Ministry of Trade, Industry, and Energy (MOTIE), Korea, under the “Regional Specialized Industry Development Program” supervised by the Korea Institute for Advancement of Technology (KIAT).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-260**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of gold nanoparticles with different size and morphologies in biological buffers

오상진 김정효[1] 이재범[2,*]

부산대학교 인지메카트로닉스공학과 [1]부산대학교 인지메카트로닉스 공학과 [2]부산대학교 광메카트로닉스공학과

The demand for biologically compatible and stable noble metal nanoparticles (NPs) has increased in recent years due to their inert nature and unique optical properties. In this article, we present 11 different synthetic methods for obtaining gold nanoparticles (Au NPs) through the use of common biological buffers. The results demonstrate that the sizes, shapes, and monodispersity of the NPs could be varied depending on the type of buffer used, as these buffers acted as both a reducing agent and a stabilizer in each synthesis. Theoretical simulations and electrochemical experiments were performed to understand the buffer-dependent variations of size and morphology exhibited by these Au NPs, which revealed that surface interactions and the electrostatic energy on the (111) surface of Au were the determining factors. The long-term stability of the synthesized NPs in buffer solution was also investigated. Most NPs synthesized using buffers showed a uniquely wide range of pH stability and excellent cell viability without the need for further modifications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-261**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

PolyMOPs : Crystallized Polymeric Metal-Organic Polyhedra

남동식 이지영 최원영*

UNIST 화학과

The metal organic polyhedra (MOPs) have potential as the supramolecular building blocks, but a few reports have explored utilizing MOPs for stepwise synthesis of extended framework. The difficulty in this building block approach is the limited synthetic strategy for interconnecting MOPs that is based on coordination-driven approach. Here, we demonstrate noble route, polymerizing MOPs, by applying condensation reaction between Zr-based MOP (UMOP-11) and flexible organic linkers. UMOP-11 is polymerized in crystalline state to form polymeric MOPs (PolyMOPs) and the PolyMOPs represent microporosity with the preserved crystallinity. This noble approach, utilizing MOP and flexible organic molecules as precursors, not only expands potential of MOP building blocks in organic synthesis but also provides promising synthetic strategy to combining metal organic materials and polymers, extensively studied for both high selectivity and processability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-262**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of Phenyl Derivatives on Mestylphenylvinyl Polysiloxane Resins

조보민 손홍래*

조선대학교 화학과

Highly refractive, thermal stable, and high transparent polysiloxane resin, mesitylphenylvinyl polysiloxane (MPVPS), has been synthesized by the thermal curing reaction of mesitylphenylvinyl oligosiloxane (MPVOS). MPVOS was obtained by a sol–gel condensation process reaction of vinyltrimethoxysilane (VTMS) and mestylphenylsilanediol (MPSD). Effect of phenyl derivatives on PVOS resins has been investigated. For the synthesis of MPVOS, MPSD instead of DPSD was used. MPVOS was thermally cured at 150 oC for 3 hr to obtain MPVPS resins. Prepared MPVPS resin showed a high refracive index of 1.56. For the comparison of DPSD, the physical properties such as an optical transmittance, refractive index, and harness were measured according to the curing time and precursor composition.This research was financially supported by the Ministry of Trade, Industry, and Energy (MOTIE), Korea, under the “Regional Specialized Industry Development Program” supervised by the Korea Institute for Advancement of Technology (KIAT).

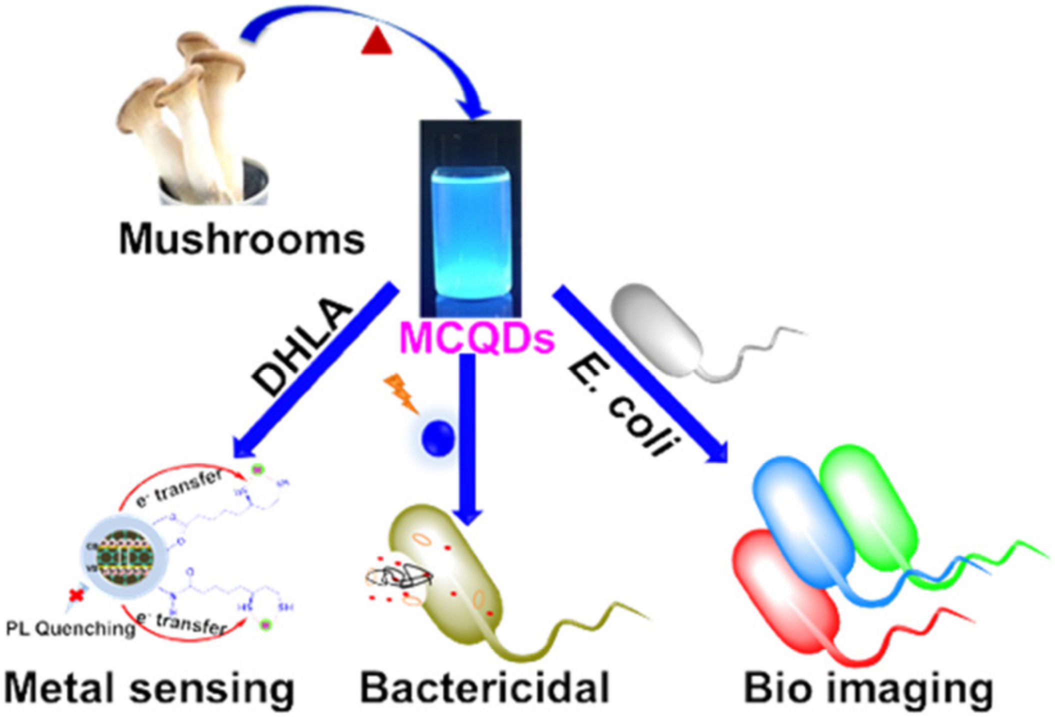
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-263**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fungal Derived High Photoluminescent Carbon Quantum Dots: Ultrasensitive Detection of Hg^{2+} Ions and Splendid Photoinduced Bactericidal Activity

SADA VENKATESWARLU 박경세[1] 윤민영*

가천대학교 글로벌캠퍼스 나노화학과 [1]군산대학교 화학과

Among all carbon allotropes, in recent years, carbon quantum dots (CQDs) continue to garner research attention due to their innumerable applications, because of their fascinating features, including superior water solubility, low cost, and unique excitation-dependent fluorescence. Most of the preparation approaches usually possess shortcomings such as the expensive and/or hazardous solvents, complex procedures, harsh reaction conditions, which restricts the availability of large-scale production of the CQDs for their potential applications. In this juncture, we synthesized amenable and oyster mushrooms (*Pleurotus*) mediated highly photo luminescent and biocompatible carbon quantum dots (CQDs). The resulting mushroom carbon quantum (MCQDs) shows high quantum yield (25 %) and exhibits stable blue fluorescence. MCQDs were applied as a effective fluorescent probe for label free sensitive detection of Hg^{2+} ions, the limits of detection was 4.13 nM. Functionalization of MCQDs with a dihydrolipoicacid acid moiety allows ultra-sensitivity for Hg^{2+} sensing as well as selectivity with the detection limit as low as 17.18 pM. In addition, the new fungal based MCQDs not only can be used for a rapid, reliable and ultra-sensitive detection of Hg^{2+} ions in real water samples, but also can act as an excellent labelling probe for bacteria with an effective photo-induced bactericidal function towards *E.coli*. The plausible results reveal that the MCQDs were highly effective in bacteria killing under visible light irradiation. These sustainable and affordable carbon materials are potentially compatible for monitoring toxic metals, and useful for visible light responsible bactericidal probe.


Mushrooms
MCQDs
DHLA
E. coli
e⁻ transfer
PL Quenching
e⁻ transfer
Metal sensing
Bactericidal
Bio imaging

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **INOR.P-264**

발표분야: 무기화학

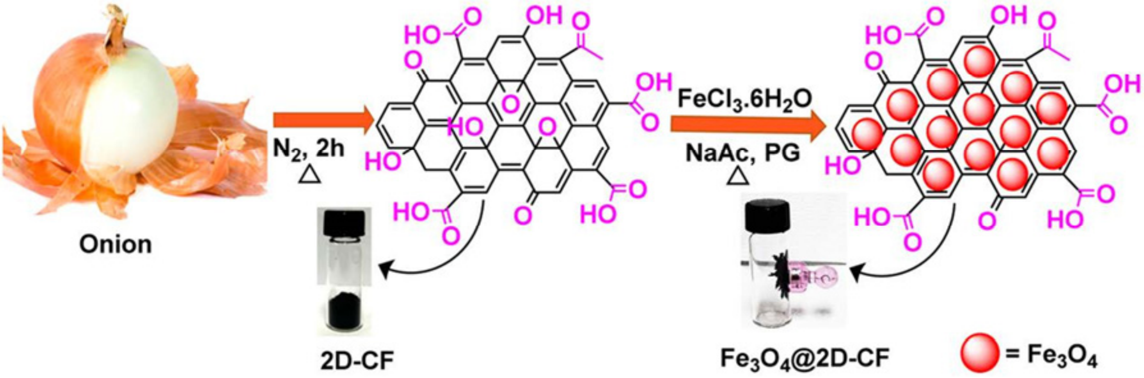
발표종류: 포스터, 발표일시: 목 11:00~12:30

Bioinspired 2D-Carbon Flakes and Fe_3O_4 Nanoparticles Composite for Arsenite Removal

SADA VENKATESWARLU* 윤민영*

가천대학교 글로벌캠퍼스 나노화학과

Development of carbon-based materials has received tremendous attention owing to their multifunctional properties. Biomaterials often serve as an inspiration for the preparation of new carbon materials. Herein, we present a facile synthesis of a new bioinspired graphene oxide-like 2D-carbon flake (CF) using a natural resource, waste onion sheathing (*Allium cep*). The 2D-CF was further decorated with crystalline Fe_3O_4 nanoparticles for applications. Superparamagnetic Fe_3O_4 nanoparticles (7 nm) were well-dispersed on the surface of the 2D-CF, which was characterized by X-ray diffractometry, X-ray photoelectron spectroscopy, Raman spectrometry, and transmission electron microscopy. Batch As(III) adsorption experiments showed that aqueous arsenic ions strongly adsorbed to the Fe_3O_4@2D-CF composite. The adsorption capacity of the Fe_3O_4@2D-CF composite for As(III) was 57.47 mg g^{-1}. The synergetic effect of both graphene oxide-like 2D-CF and Fe_3O_4 nanoparticles aided in excellent As(III) adsorption. An As(III) ion adsorption kinetics study showed that adsorption was very fast at the initial stage, and equilibrium was reached within 60 min following a pseudo-second-order rate model. Owing to the excellent superparamagnetic properties (52.6 emu g^{-1}), the Fe_3O_4@2D-CF composite exhibited superb reusability with the shortest recovery time (28 s) among reported materials. This study indicated that Fe_3O_4@2D-CF composites can be used for practical applications as a global economic material for future generations.


Onion
N_2, 2h
△
2D-CF
$FeCl_3.6H_2O$
NaAc, PG
△
Fe_3O_4@2D-CF
= Fe_3O_4

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-265**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal-Organic Nanococoons for Selective CO_2 Adsorption

이수찬 최원영*

UNIST 화학과

Releasing carbon dioxide (CO_2) generated from the continual burning of fossil fuels has emerged as a main culprit. Porous materials such as metal-organic frameworks (MOFs), zeolites, porous organic polymers, and organic cages are identified as key candidate materials for potential CO_2 capture. However, CO_2 sorption study of 0-D metal-organic molecules is underexplored. Presumably, polar CO_2-philic environment such as sulfonyl ($-SO_2-$) or sulfonated ($-SO_3H$) groups should have a positive effect on increasing CO_2 adsorption capacity. Nevertheless, the treated polar functional groups could not lead to maintain the crystalline structure and enhance porosity in metal-organic molecules. Herein, we present robust Zr(IV)-based metal-organic nanococoons with solubility in polar solvents. By modulating bridge atom functionality of two types V-shaped linkers, 4,4'-sulfonyldibenzoic acid (SDB) and 4,4'-methylenedibenzoic acid (MDB), UMOM-3 and UMOM-4 are synthesized and we introduce enhanced gas sorption property and structural improvement.UMOM-3 has the noticeable porosity, structural integrity and enhanced CO_2 adsorption capacity over UMOM-4 from $-SO_2-$ moiety. Furthermore, UMOM-3 reveals the great 15:85 CO_2 over N_2 selectivity (64), which is the highest value in cage structures and sulfonyl group contained MOFs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-266**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Solid-acid ZrO_2/SO_4^{-2} for Composite Polymer Electrolyte Membrane for Fuel Cells

이용미 Md. Aminur Rahman[1] 한옥희[2,*]

충남대학교 분석과학기술대학원 분석과학기술학과 [1]충남대학교 분석과학기술대학원 [2]한국기초과학지원연구원 서울서부센터

Polymer electrolyte membrane fuel cells (PEMFCs) are very promising as electrochemical power sources for application in portable devices and transportation, due to their high energy conversion efficiency with low environmental impact. When PEMFCs operate at the temperature above 80℃, PEMFCs' ionic conductivity drastically decreases due to the evaporation of the moisture. To solve this problem, composite membranes containing inorganic fillers with the high water uptake and high acid concentrations have been developed. Composite membranes containing finely dispersed hygroscopic inorganic oxides such as SiO_2, TiO_2, ZrO_2 and the inorganic oxides modified with SO_4^{-2} ($MO_2/SO_4^{-2}$where M = Si, Ti, or Zr) show improved water retention properties and, consequently, suitable proton conductivity even at high temperatures. Because, among the oxides, ZrO_2 is more stable at high temperatures and has better conductivity and ductility, it has been used as a filler to polymer electrolyte membranes for the fuel cells operated in the harsh environments such as high temperature and pressure. In particular, ZrO_2/SO_4^{-2} has strong acidity and water affinity resulting in promoting the local protonic migration in the Nafion-based composite PEMs because ZrO_2/SO_4^{-2}has the best activity and spatial distribution of sulfate ions compared to SiO_2/SO_4^{-2} or TiO_2/SO_4^{-2}. In addition, price of ZrO_2 is only ~1/3 of that of TiO_2 brookite with the similar properties.In this study, we aim to find out optimum mole ratios of ZrO_2 and SO_4^{-2} to prepare ZrO_2/SO_4^{-2} of the best proton conductivity and water retention. We have compared the properties of ZrO_2/SO_4^{-2} synthesized by mixing ZrO_2 nano-powder and $(NH_4)_2SO_4$ or H_2SO_4 solution at the mole ratio of 1:0.5, 1:1, 1:2, 1:3, 1:4, and 1:5. The synthesized ZrO_2/SO_4^{-2} was calcined at 350℃~550℃ for 10 h and then cooled for 12 h. We have determined the amount of SO_4^{-2} in the ZrO_2/SO_4^{-2} by tritrating with 0.005 M NaOH solution. The surface of the ZrO_2/SO_4^{-2} powder will be characterized with Automatic Elemental Analyzer and SEM-EDS and TEM, and the composite polymer electrolyte membranes with Nafion and ZrO_2/SO_4^{-2} will be prepared.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-267**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Novel Bidentate Ligands for N-Coordinated Metal Complexes as ALD/CVD Precursors

이가연 정택모[1] 김창균[2] 박보근[1] 전동주[3,*]

한국화학연구원 박막재료연구센터 [1]한국화학연구원 화학소재연구본부 박막재료연구센터 [2]한국화학연구원 화학소재연구본부 [3]한국화학연구원 화학물질연구단

New precursors have been continuously required for metal and metal oxide thin films which diverse applications to electronic devices. For the metal precursors having desirable properties, we designed new ligands with two concepts, firstly, a chelation effect through an electron donor functional group containing nitrogen and oxygen atom, secondly, introduction of bulky substituents such as dialkyl moiety at the position of hydroxyl group, which prevents the interaction between molecules, thereby, it was expected the formation of a monomer complex having high vapor pressure. We have studied the synthesis of methoxymethylaminoalcohol-type, N,N-dimethylaminoamine-type and N-methylaminoalcohol-type organic ligands, and of them, methoxymethylaminoal -cohols were used for the preparation of new Tin and Germanium precursors. Four complexes were characterized by IR, 1Hand13C NMR,EA,and the solid structure were respectively confirmed by X-ray single crystallography as a monomer showing a distorted trigonal bipyramidal at a metal center.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-268**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Sensing of Nitro Aromatic Explosives Using In-MIL-53-NH_2 MOF

Sharma Amitosh 성준모[1] 임재웅[2] 나명수[1,*]

UNIST Chemistry [1]UNIST 화학과 [2]UNIST 분자과학부

Analogous MOF of MIL-53 has been synthesized using indium $In(NO_3)_3 \cdot XH_2O$ and amino-terepthalic acid. SC-XRD study shows the structure similarity to MIL-53 series. Synthesized MOF has been characterized by IR, PXRD and TGA. This MOF shows sensing ability towards nitro aromatic explosives by fluorescence quenching phenomenon.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-269**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Multiplexed biomolecule detection dynamic interaction between plasmonic nanoparticles on lipid bilayers

김선기 남좌민*

서울대학교 화학부

Monitoring single nanoparticle interactions is important for many complex biochemical and physical processes, yet it remains challenging for conventional methods with limited applicability. Recently, we developed a plasmonic nanoparticle-modified supported lipid bilayer (PNP-SLB) platform for observing dynamic interaction between plasmonic nanoparticles in real-time [1]. Plasmonic nanoparticles are tethered to the supported lipid bilayers which provide two-dimensional fluidic surface with controllable mobility. Massively parallel nanoparticle interactions were monitored quantitatively in single nanoparticle resolution by dark-field microscopy. In this study, we induced dynamic interaction between plasmonic nanoparticles for multiplexed detection of biomolecules. Different assembly mode between nanoparticles can be differentiated and quantitatively measured. References 1.Y. K. Lee, S. Kim, J.-W. Oh and J.-M. Nam, J. Am. Chem. Soc. 136, 4081 (2014).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **INOR.P-270**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tuning Rectification by the Controlled Use of Different-Sized Diluents in Heterogeneous Self-Assembled Monolayers

조수진 공규돈 김미소 윤효재*

고려대학교 화학과

For studies of organic and molecular electronics, eliminating structural defects in molecular components inside devices is usually needed for improving their performance. This presentation shows that this bother can be turned into a strength for modulating the performance of devices. A monolayer of an organic rectifier, 2,2′-bipyridine-terminated n-undecanethiolate, is systematically diluted with electronically inactive diluents, n-alkanethiolates of different lengths. Such a dilution leads to remarkable gradients of rectification in a range of approximately two orders of magnitude, retaining its polarity. Trends of rectification against the length of the diluent indicate the gradient of rectification is extremely sensitive to the molecular structure of the diluent. Further studies reveal that noncovalent intermolecular interactions within monolayers result in finely tunable gradients of structural defect and rectification.

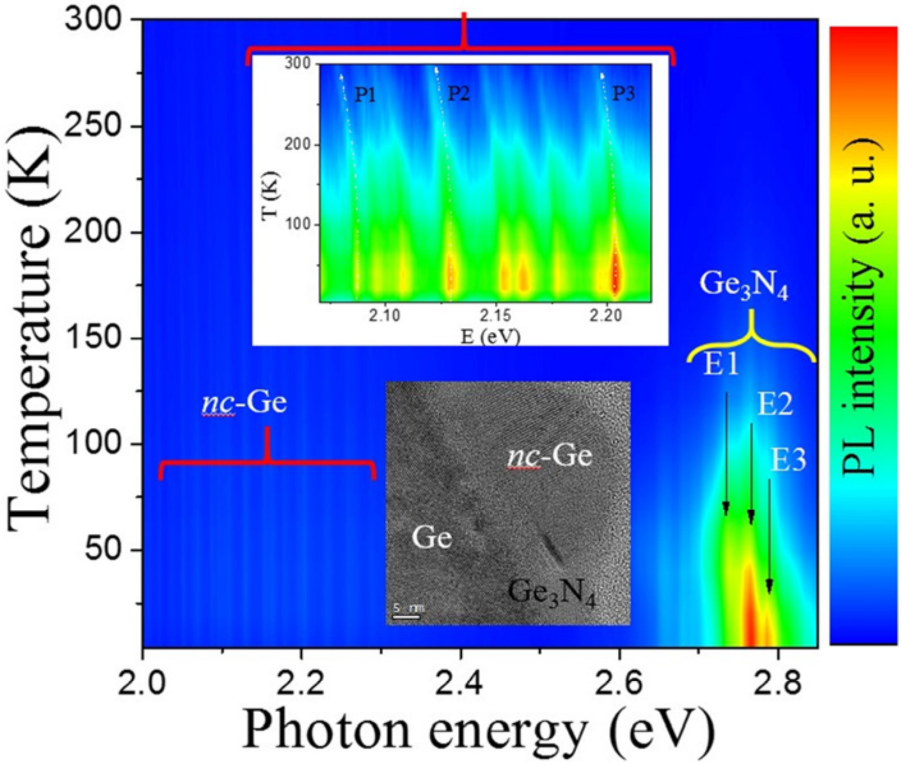
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-271**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Carrier trapping and confinement in Ge nanocrystal surrounding layer of Ge_3N_4 by N_2^+ ion implantation on Ge(111) and rapid thermal annealing

이영미[*] Christopher C. S. Chan[1] Benjamin P. L. Reid[1] Luke Nuttall[1] Robert A. Taylor[1]

포항가속기연구소/포항공대 10D beamline [1]University of Oxford

Semiconductor nanostructures are arguably the most promising technology for future optoelectronics and memory device applications due to the recent rapid advances in nanoscale science and technqiues. Ge nanocrystal (*nc*-Ge) is an attractive materials for application of electronic and optical devices due to its superior charge storage performance as well as optical luminescence. Ge is an indirect gap semiconductor, with two main electronic transitions, the first at 0.67 eV (indirect) the second at 0.8 eV (direct) and *nc*-Ge are one of the candidates for such applications due to their superior charge storage performance. Here, we present the formation of *nc*-Ge surrounded by Ge_3N_4 and its optical properties. The *nc*-Ge were prepared by N_2^+ ion implantation on Ge (111) single crystal and perfectly surrounded by a Ge_3N_4 confirmed by measuring the high-resolution transmission electron microscopy (HRTEM). The high-resolution x-ray photoelectron spectroscopy (HRXPS) with the synchrotron radiation characterizes the existence of the Ge_3N_4 which can structurally confine the Ge nanocrystal. Individual PL peaks are finely resolved with our micro-PL system, attributed to emission of the *nc*-Ge. These peaks are shown to be behave with excitonic characteristics and we argue that the spread of *nc*-Ge peaks in the PL spectrum are due to different confinement energies arising from the variation in size of the nanocrystal.


300
250
200
150
100
50
Temperature (K)
2.0
2.2
2.4
2.6
2.8
Photon energy (eV)
PL intensity (a. u.)
300
200
100
T (K)
P1
P2
P3
2.10
2.15
2.20
E (eV)
nc-Ge
nc-Ge
Ge
Ge_3N_4
5 nm
Ge_3N_4
E1
E2
E3

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-272**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical reaction path for elimination of NH_3 by aniline from Ir pincer type complex of amido hydride

장효원

순천대학교 화학과

We propose theoretical reaction path for the experimental observation of ammonia elimination from 16-electron species of $[\kappa^3\text{-}(2\text{-}Cy_2\mathit{P}C_6H_4)_2\mathit{Si}\ Me]Ir(H)(NH_2)$ by aniline.We find that a favorable reaction path involves 18-electron species of aniline adduct to reactant complex, hydrogen transfer between nitrogen centers, and the ammonia dissociation from the resulting amine adduct.Therefore, reductive mechanism is not involved during ammonia elimination, also the hydride ligand remains intact throught the whole process.In short, the key step can be designated as hydrogen transfer between aniline and amido ligands.Finally, the calculated free energy barriers indicate the overall reaction may be facile.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-273**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A DFT Study on the Formation of Hemicucurbit[6]uril by Step-Growth Oligomerization and End-to-End Cyclization

강영기* 유인기

충북대학교 화학과

The formation of hemicucurbit[6]uril (hCB[6]) from ethyleneurea with formaldehyde in acidic aqueous solution was explored by the step-growth oligomerization of acyclic methylene-bridged ethyleneurea oligomers and the end-to-end cyclization of hexamer using density functional methods and the implicit solvation model in water. The oligomerization and cyclization barriers were approximately half lower than that of the final step of iminium formation, and all product complexes were more stable than the corresponding reactant complexes. Thus, the formation of hCB[6] is kinetically and thermodynamically favored in acidic aqueous solution. In particular, the "alternate" conformation of hCB[6] is enthalpically and entropically preferred over the "cone" conformation, which is consistent with the crystal structure of hCB[6].

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-274**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anomalous Dynamics of Water Confined in Hydrophilic Protein–Protein Interface

정성호 함시현*

숙명여자대학교 화학과

Confined water often exhibits anomalous properties not observable in the bulk phase. Although water in hydrophobic confinement has been the focus of intense investigation, the behavior of water confined between hydrophilic surfaces, which are more frequently found in biological systems, has not been fully explored. Here, we investigate using molecular dynamics simulations dynamical properties of the water molecules located at a hydrophilic protein–protein interface. We find that those water molecules exhibit glassy slow relaxations even at 300 K. In particular, the rotational dynamics show a logarithmic decay that was observed in glass-forming liquids at deeply supercooled states. We argue that such slow water dynamics are indeed induced by the hydrophilic binding surfaces, which is in opposite to the picture that the hydration water slaves protein motions. Our results will significantly impact the view on the role of water in protein–protein interactions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-275**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Understanding the Stability of Human Telomeric G-quadruplexes by Molecular Dynamics Simulations

이진경 함시현*

숙명여자대학교 화학과

Guanine-rich regions in DNA called G-quadruplexes, which are of recent biological interest since they are considered as potential anticancer drug targets. While several different topologies (parallel, antiparallel, mixed-hybrid 1 and mixed-hybrid 2) are known for the G-quadruplex structures, the relative stability of those structures remains elusive. Here we investigate the molecular origin of the stability of Human telomeric G-quadruplexes to know the conformational preference, with quantum mechanical calculations and molecular dynamics simulations. The effect of ions (Na+, K+) upon complexation in water is also quantified by the solvation free energy calculations based on the integral-equation theory. Thereby, we discuss the conformational preference and the effect of solvent upon Human telomeric G-quadruplexes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-276**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation of CeO_2/Ce_2O_3 nano-hybrid by using pulsed laser ablation in water

마로리 김태규* **ISLAMMOHAMMADJAHURUL devulapalliamaranathareddy**

부산대학교 화학과

Cerium-based nanohybrids have attracted considerable attention in photocatalytic research owing to their remarkable potential for the photodegradation of environmental pollutants. However, formation process of nanohybrid suffers from complex operations with specialized equipments, extreme conditions, long term durations and low yields which make them infeasible for efficient ultilization. In this study, we are first time to introduce the pulsed laser ablation in liquid phase (PLAL) for the synthesis of oxygen vacancy affluent CeO_2/Ce_2O_3 nanohybrids, which is an alternative to the hydrothermal as well as calcination methods. The microstructures and optical properties of the nanocomposites are charaterized by TEM, XRD, XPS and DRS analysis. The photocatalytic activity of CeO_2/Ce_2O_3 nanohybrid showed superior MB dye degradation rate than that of bare CeO_2 nanostructures. The enhanced performance of CeO_2/Ce_2O_3 elucidated through oxygen vacancy driven Z-scheme mechanism, where efficient separation of the photogenerated charge carriers significataly contributed for phtocatalytic enhancement; this was further evident by both PL and scavenger experimental results. Moreover, the synthesized CeO_2/Ce_2O_3 nanocomposites exhibit a strong blue emission, which can be taken advantages for the development of potential LED manufacturing.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-277**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Context-Dependent Effects on Hydrophobicity of Amino Acids in Protein

조한울 함시현*

숙명여자대학교 화학과

Hydrophobicity is the important concept to understand the role of water in protein folding, protein aggregation, and protein-protein interaction. Conventionally, the hydrophobicity of a protein is debated based on the hydrophobicity scales determined for individual free amino acids, assuming that they are unaltered when they are embedded in a protein. Here, we quantify the protein hydrophobicity by computing the solvation free energy and decompose it into the contributions of each residues. We find that the hydrophobicity of residues is significantly affected by the secondary structure formation such as alpha helix, beta sheet. Also, we observe that tendency of hydrophobicity of neutral polar residues is a bit different from that of nonpolar residues. Based on the correlation between residual hydrophobicity and solvent accessible surface area of residue, we discuss the factors to contribute residual hydrophobicity when amino acid is embedded in a protein. Our results provide the valuable for understanding functions of protein on the basis of hydrophobicity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-278**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular Insights into Fasciclin 1 Domain 4 and Its Disease-Related Mutants: A Computational Study

조선희 함시현*

숙명여자대학교 화학과

Human fasciclin 1 domain 4 (FAS1-4) is an extracellular domain whose main function is cell adhesion through an interaction with integrin. Aggregation of mutated FAS1-4 is the major cause of corneal dystrophy diseases which results in a reduction of visual power and in eventual blindness. However, structural information of the mutants of this protein at atomic level remain elusive. Herein, we performed molecular dynamics (MD) simulations and hydration thermodynamic analysis to characterize the wild type FAS1-4 and its three mutants (A546T, R555Q and R555W). We focused on investigating the structural features responsible for cell adhesion function and the corresponding thermodynamic features of these proteins to characterize the aggregation-prone nature of the respective mutants. Our results provide the structural and thermodynamic features on wtFAS1-4 and its mutants, which will contribute to understand the molecular mechanisms in FAS1-4 aggregation related to corneal dystrophy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-279**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Elucidating Aggregation-Prone Characteristics of Tau43 Protein with Molecular Dynamic Simulation and Solvation Thermodynamic Analysis

BUI THI DIEM HUONG 함시현*

숙명여자대학교 화학과

In Alzheimer's disease and other dementias, Tau protein dissociates from the axonal microtubule and abnormally aggregates into paired helical filaments (PHFs). However, the molecular details of tau aggregation propensity is largely unknown. In this study, we have performed multiple all-atom, explicit-water molecular dynamics simulations followed by solvation thermodynamic analyses on the 43-residue fragment of human tau protein (termed Tau43) comprising the third repeat of tau plus some flanking residues to characterize its structural and thermodynamic properties. Tau43 monomer exhibits fairly localized β-sheet structure, extended hydrophobic surface and the increased solvation free energy. Based on site-directed thermodynamic analysis, we also elucidate Lysine as well as hydrophobic residues' contribution to the total solvation free energy. Our analyses thus identify the structural and thermodynamic features of the Tau43 monomer that potentially seed the aggregation process in water.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-280**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Application of the Extended Grunwald-Winstein Equationto the Solvolysis of Diphenylacetyl Chloride

고한중

전주교육대학교 과학교육과

This report shows the rates of solvolyses for diphenylacetyl chloride in ethanol, methanol, aqueous binary mixtures incorporating ethanol, methanol, acetone, 2,2,2-trifluoroethanol, and 1,1,1,3,3,3-hexafluoro-2-propanol, and binary mixtures of TFE with ethanol are reported. The kinetic data obtained from the reactions in 34 different solvents and solvent mixtures gave an extended Grunwald-Winstein correlation with the l value of 0.76, the m value of 0.34. The appreciable values for both l and m suggest that the bond formation is ahead of the bond breaking with an SN2 mechanism, and the l/m ratio of 2.2 is also in the range of values found for SN2 reaction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-281**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical Investigation for the Reaction Pathway from Acetylene to Naphthalene with La Atom via La-Activated Bicyclo-Oligomerization

문지원 김중한*

가톨릭대학교 화학과

Transition metal-activated bicycle-oligomerization is an important technique to construct ring compounds in organic system. A recent experimental study of La-activated acetylene bicycle-oligomerization to form naphthalene in the gas phase was performed using time of flight (TOF) mass spectrometry and mass-analyzed threshold ionization (MATI) spectroscopy. However, the detailed reaction mechanism is still unknown. We investigated the reaction potential energy surfaces (PESs) which include sequential acetylene addition and dehydrogenation. The molecular structures of reactant, transition states, intermediates, and products were optimized using the density functional theory (DFT) method. The minima and transition states were confirmed using the intrinsic reaction coordinate (IRC) method. The single-point calculations using the coupled-cluster single and doubles with perturbative triples (CCSD(T)) were also performed to obtain accurate energetics. We suggest the favourable reaction pathways from acetylene with La atom to naphthalene and they are in consistent with the experimental observations.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-282**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Benchmark Study of Performance of Density Functional Theory for Molecular Properties of Li_2S_n (n=1~8) clusters

채명주 문지원[1] 김중한[1,*]

가톨릭대학교 자연과학부/화학과 [1]가톨릭대학교 화학과

The cathode redox reactions in the lithium-sulfur battery involve various types of Li_2S_n (n=1~8) clusters. However, their detailed molecular structures are still unknown. Therefore, we investigate the molecular properties of Li_2S_n (n=1~8) clusters using high-level ab initio method such as the coupled-cluster singles and doubles with perturbative triples (CCSD(T)) method. The benchmark study of performance of density functional theory (DFT) to calculate the molecular properties of Li_2S_n (n=1~8) clusters was also performed. DFT functional which well reproduces the results of CCSD(T) has been proposed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-283**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Morphology-Controlled Synthesis of ZnS Nanostructures: Tunable Photoluminescence in the Visible Region and Photocatalyst for Laser-Induced Efficient Reduction of Cr(VI)

김유진 **devulapalliamaranathareddy** 박한빛 김태규*

부산대학교 화학과

Developing a green and convenient synthesis process for control of the morphology of ZnS nanostructures is of great interest but remains a grand challenge. Therefore, a strategy for tuning the morphology of ZnS nanostructures using different anionic precursors without addition of any organic surfactants or templates is proposed. The role of anionic precursors in determining the morphologies and possible growth mechanism are proposed to involve oriented aggregation and the Ostwald ripening process. The as-synthesized ZnS nanostructures also exhibited outstanding tunable photoluminescence in the visible region, depending on the morphology and excitation wavelength. Moreover, the influence of the morphology of the ZnS nanostructures on the photocatalytic reduction of Cr(VI) in water under pulsed laser irradiation was investigated. The analysis revealed that rice grain shaped ZnS nanostructures exhibit more efficient photocatalytic activity for Cr(VI) reduction compared to other nanostructures. We also investigated the dependence of the rate of Cr(VI) reduction on the pulsed laser power, pH, and Cr (VI) concentration. The work present provides a new approach for designing ZnS nanostructures with different morphologies for application in light emitting diodes (LEDs) and water purification systems.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-284**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Zeolitic imidazolate framework-67 (ZIF-67) rhombic dodecahedrons as full-spectrum light harvesting photocatalyst for environmental remediation

김태규* 박한빛 **devulapalliamaranathareddy** 김유진

부산대학교 화학과

The inferior utilisation efficiency of light is the main obstacle to the practical application of traditional photocatalysts like TiO_2 and ZnO. Therefore, the development of novel photocatalysts with the capability of harvesting full spectrum light (from UV to near-infrared (NIR)) energy is a promising solution for solar energy conversion and environmental remediation. Here we report the discovery of a single material that can harvest UV, visible (VIS), and NIR radiations to decompose heavy metal contaminants in aqueous solution. Zeolitic imidazolate framework-67 (ZIF-67) rhombic dodecahedrons were synthesised through a facile solution approach and employed in the reduction of Cr(VI) under UV−VIS−NIR pulsed laser irradiation, which was generated from the fundamental, second and third harmonics of Nd:YAG laser, respectively. The nanostructures showed efficient Cr(VI) reduction under UV, Vis, and NIR laser irradiation and the measured reduction efficiency (%) was 71.22%, 69.52%, and 40.79%, respectively after 120 min. A possible explanation for the photocatalytic activity in Cr(VI) reduction was proposed. This is the first study of its kind where pulsed laser and ZIF-67 rhombic dodecahedrons capable of harvesting full spectrum light energy have been employed for the removal of Cr(VI) from water. The extraordinary capacity of harvesting full-spectrum light and long-term stability make ZIF-67 a potential photocatalyst for environmental remediation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-285**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cobalt phosphide with CdS/RGO-MoS_2 nonacomposites as a nobel metal free catalyst for hydrogen production from water

이승희 홍상엽 devulapalliamaranathareddy 김태규*

부산대학교 화학과

Commercial applications of sustainable photocatalytic hydrogen production via water splitting, an important future source of renewable energy, are interrupted by the high cost and scarcity of the requisite noble metal co-catalysts. This problem could be overcome by developing highly active and durable noble-metal-free photocatalysts. A new solar-light-active noble-metal-free catalyst featuring dandelion-flower-like cobalt-phosphide embedded with CdS nanostructures grown on reduced graphene oxide (RGO)-MoS_2 nanosheets was designed, and its photocatalytic hydrogen production activity was evaluated in water under simulated sunlight irradiation using lactic acid as a sacrificial reagent. The results show that the optimized CdS/RGO-MoS_2 @CoP photocatalyst exhibited an efficient H_2 production rate of 83907 μmol h^{-1} g^{-1} with an apparent quantum efficiency of 22.5%, far exceeding those of bare CdS (1053 μmol h^{-1} g^{-1}), CdS-RGO (12177 μmol h^{-1} g^{-1}), CdS-RGO-MoS_2 (29268 μmol h^{-1} g^{-1}), CdS:CoP (32606 μmol h^{-1} g^{-1}), CdS/CoP-RGO (54259 μmol h^{-1} g^{-1}) and CdS:Pt (12478 μmol h^{-1} g^{-1}) nanostructures. The proposed mechanism for the enhancement of the photocatalytic hydrogen evaluation rate of CdS/MoS_2 -RGO@CoP is based on the efficient separation of photogenerated electron–hole pairs. In the nanocomposite, the wrapped RGO nano-sheets serve as good electron collectors and transporters. Meanwhile, the MoS_2 and CoP nanostructures serve as a co-catalyst and electron acceptor, respectively, for the effective separation of the photo-charge carrier from the bare nanostructures, thereby decreasing the probability of electron–hole recombination at the interface of the nanocomposites and further stimulating the surface H_2 production kinetics.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-286**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Resummation of the Brillouin-Wigner perturbation series

이승훈 이상엽*

서울대학교 화학부

We present a new method of resumming the Brillouin-Wigner perturbation series with Epstein-Nesbet partitioning. Both the nondegenerate and quasi-degenerate cases are considered. We illustrate the accuracy of the proposed resummed Brillouin-Wigner perturbation theory for selected atoms and small molecules, as well as a simple model system like the quartic anharmonic oscillator. For the electronic structure problems, it is found that the present theory provides essentially the same results as the corresponding configuration-interaction calculations at the level of the fourth-order calculations.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-287**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ab initio study on anomalous structures of [(N-heterocycle)-CO_2]$^-$ complex

오레나 임은학 허지영[1] 김성근[*]

서울대학교 화학부 [1]상명대학교 의생명공학과

Although CO_2 has a negative adiabatic electron affinity, it forms a stable anionic complex with many N-heterocycles (NHCs) by taking up a partial negative charge as in the well-known case of [pyridine-CO_2]$^-$. Here, we report an anomalous group of [NHC-CO_2]$^-$ complexes that are more stable in the orthogonal geometry than in the coplanar one as the CO_2 moiety is rotated internally around the molecular plane of NHC. The culprit for this seemingly anomalous case is explained by the steric effect and the electron affinity of NHCs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-288**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

DC-TOF 업그레이드 : 실시간-실상황 분광법

소지용

한국원자력연구원 중성자과학부

Disk chopper-time-of flight spectrometer (DC-TOF)는 한국 유일의 중성자 산란 시설인 하나로의 냉중성자 실험동에 설치된 비탄성/준탄성 산란장치이다. 50 ueV~50 meV 의 에너지 영역에서의 준탄성/비탄성 산란 측정을 통해 다양한 분자/원자의 동역학을 측정 할 수 있으며, 현재 4 K ~ 450 K 의 온도 영역에서 측정을 할 수 있다. 2012 년 첫번째 빔 입사에 성공했으며 2014 년 이용자에게 개방되었다. 2016 년 하반기로 예정된 하나로 재가동 시점에서 이용자들이 사용 할 수 있다.외국의 중성자 시설에서는 유사한 장치를 이용하여 유기분자나 나노분자에서부터 초전도체, 자성체, 고분자, 생체분자등 다양한 물질의 동역학을 연구하고 있다. DC-TOF 는 그동안의 시험과정에서 외국 장치와 경쟁할 수 있음을 확인하였다. 본 발표에서는 현재 추진중인 DC-TOF 의 실시간-실상황 분광법에 대해 소개하고 이를 이용하여 다양한 물리/화학적 반응을 연구하는데 사용될 수 있음을 설명하고자 한다.

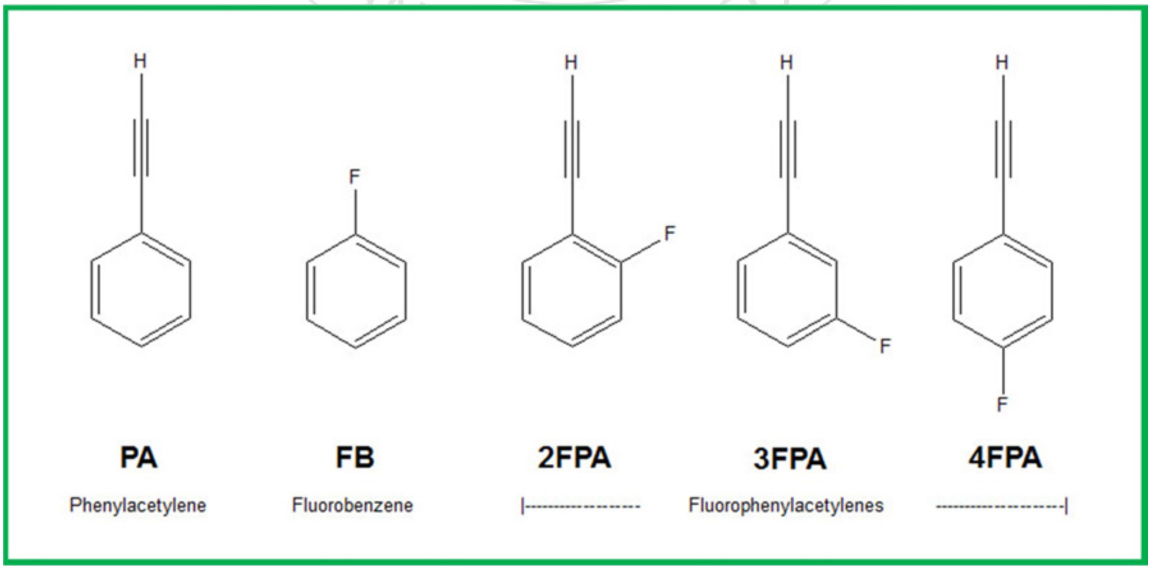
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-289**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Microwave and *ab initio* studies on the molecular structure and dipole moments of Fluorophenylacetylenes (FPAs)

장희수 오정진*

숙명여자대학교 화학과

The analysis of microwave spectrum for the normal and carbon-13 isotopic species, measured by a chirped-pulse (CP) and a cavity resonance Fourier transform microwave spectrometer (FTMW), determined experimental substitution (r_s) and least-squares fitting (r_0) structures of fluorophenylacetylenes (3FPA and 4FPA). Rotational constants, quartic centrifugal distortion constants, and ring geometry for the parents were compared to those of the equilibrium structures (r_e) optimized at the MP2 level with the 6-311++G(2d,2p) basis set. In addition, experimental dipole moment components derived from the measurement of Stark shift in their rotational transitions. They were in good agreement with results from the *ab initio* calculation.



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-290**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

In Silico Investigation of the Structural and Thermodynamic Differences of Aβ42 and Aβ40 in Predominantly Aqueous Environment

CHATTERJEE PRATHIT 임해리 함시현*

숙명여자대학교 화학과

The self-aggregation of amyloidβ (Aβ) peptides continues to be an intriguing problem, because of their diverse implications in Alzheimer's and other neurodegenerative diseases. Among the different variants of Aβ peptides, Aβ40 and Aβ42 are abundantly present in physiological systems. Aβ42 exhibits greater aggregation propensity relative to Aβ40 in spite of their nearly identical sequential pattern, the former contains additional I41A42 residues in the C-terminal region. Our present results, obtained from atomistic molecular dynamics simulations, depict no distinguishable differences in structural propensity between the two variants, in accordance with recent NMR results. Rather, the differences are found to originate from the solvation thermodynamics between the two variants, based on our solvation thermodynamic analyses. The decomposition analyses of solvation free energy indicate that the C-terminal region of Aβ42, along with the salt-bridge promoting charged residues, increases the overall solvation free energy. The increased solvation free energy for Aβ42 therefore indicates that the corresponding variant is more hydrophobic in aqueous environment, due to inclusion of two additional hydrophobic residues (I41A42) in the C-terminal region, as well as electrostatically driven increased salt-bridge formation propensity. This implies a potential water assisted promotion of intermolecular interaction between the monomeric peptide units of Aβ42, thereby leading to self-aggregation.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-291**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Nonadiabatic Molecular Dynamics of Dimethylnitramine

RashidMdAlMamunur 최철호[1,*]

경북대학교 일반대학원 화학과 [1]경북대학교 화학과

Since the photodecomposition of energetic materials is an extremely complicated reaction, the mechanisms and dynamics of the dominant decomposition reactions are still a challenge. Dimethylnitramine, as one of the simplest compounds in the nitramine family, which attracted broad research interest in the energetic materials sector, has been used in the investigation of the unimolecular decomposition mechanism. Based on the reported results, most scientists supported NO2 elimination as the major decomposition channel of dimethylnitramine from excited states, but inconsistencies still existed between the nitro-nitrile isomerization and NO2 elimination mechanisms. To understand about the photoinduced excited-state nonadiabatic processes and successive unimolecular dissociation of dimethylnitramine, we applied nonadiabatic molecular dynamics using Tully's Surface Hopping method. We observed that conical intersection plays an essential role for the ultrafast internal conversion from excited state to ground state in the initial steps of the decomposition of dimethylnitramine. Pyramidalization/bending motion of N-NO2 moiety are associated with the surface hopping followed by dissociation dynamics of dimethylnitramine. We found NO2 elimination as the major decomposition channel of dimethylnitramine through an N-N bond fission mechanism. Some evidence of minor decomposition pathway was also found with the initial elimination of O with formation of nitrosamine.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-292**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Single-molecule study on guide RNAs as structural regulators for the activation of Cas9 endonuclease

성기원 박소영 김진수 배상수[1] 김성근[*]

서울대학교 화학부 [1]한양대학교 화학과

The type II CRISPR-Cas system that consists of Cas9 endonuclease and two guide RNAs (gRNAs), tracrRNA and crRNA, recognizes and cleaves target DNA in what is thought to have derived from a bacterial adaptive immune mechanism against invading viruses and plasmids. Here, we report the structural roles of the two guide RNAs in the activation of Cas9 endonuclease, studied by pseudo-ensemble and single-molecule fluorescence assays. The tracrRNA plays an important role in the formation step of the catalytically active Cas9-gRNA complex. It leads Cas9 preferentially toward a folding pathway for nuclease activity over other pathways leading to a deactivated structure newly discovered in this study. After the Cas9-gRNA complex binds the target DNA, R-loop expansion between crRNA and the target DNA shows intrinsically repetitive transitions between two distinct sub-structures termed 'open' and 'zipped' conformations. This dynamic, crRNA-related conformational change is found to control the nuclease activation of Cas9 by allowing the DNA cleavage reaction only when the zipped conformation is formed. These results provide a mechanistic insight into how both tracrRNA and crRNA structurally regulate the DNA cleavage activity of Cas9 endonuclease to minimize the off-target effects.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-293**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of ZnO nanoparticle on FTO substrate by using various of amine for self-cleaning ability and anti-reflective property

유정열 김우석 이얼 정동기 이유로 김재욱 김종규*

단국대학교 화학과

In this study, ZnO nanoparticle(NP) has been synthesized on the FTO substrate by using sol-gel coating and hydrothermal method for producing a film which has self-cleaning and anti-reflective properties. When growing ZnO by hydrothermal method, a variety of amine was used to study the effect of the amine. The properties of synthesized material were studied with different devices. The structural properties have been identified through X-Ray Diffraction(XRD), Field-Emission Scanning Electron Microscopy(FE-SEM), while UV-Vis spectrometer and Contact Angle analyzer have conducted for the anti-reflective properties, hydrophilicity and self-cleaning ability. The structure of synthesized ZnO NP indicates in hexagonal wurzite. Various shape of ZnO observed by FE-SEM. The anti-reflective properties have been confirmed through measurement of the transmittance. Contact angle analyzer observes the material's wettability, which is an important factor for hydrophilicity. ZnO NP array FTO film exhibits excellent photocatalytic activity.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-294**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ultrafast Photodissociation of nitric oxide from S-nitrosothiols

이소현 임만호* 박성철

부산대학교 화학과

일산화질소는 생체에서 중요한 기능을 하는 분자이며, 특히 세포 간 신호 전달 물질로써 많이 작용한다. 또한 NO 는 많은 염증 질환의 병리학과 암이나 당뇨병, 신경 퇴행성 질환과 같은 다양한 병리학적 조건들과 관련이 있다.다양한 요인에 의해 NO 를 방출하는 많은 분자들이 존재하는데, 이 때 단백질 활성 자리의 NO 결합에 대한 동역학은 생리학적인 과정에서 단백질의 기능과 반응 메커니즘을 완전히 이해하는 데 필수적이다.특히 L-시스테인의 분자 구조에서 찾아 볼 수 있는 황은 NO 와 결합하고 떨어지는 과정에서 주된 역할을 한다. 우리는 이러한 단백질과 유사한 형태의 알킬 아질산염(RSNO), 그 중에서도 비교적 반감기가 긴 일차 구조 화합물들을 합성하고 시분해능 적외선 분광기를 이용해 NO 의 초고속 동역학에 대해 분석해보았다.비교에 사용한 각각의 S-nitrosothiol 은 1500 cm^{-1} 대 에서 방출, 1800 cm^{-1} 대 에서 흡수를 보였다. 1500 cm^{-1} 에서 나타나는 표백(bleaching) 신호는 NO 의 진동 때문에 나타나게 되는데, 이 때 나타나는 신호에서 trans 와 cis 형태의 이성질체를 관찰 할 수 있었다. 알킬 아질산염의 구조에서 NO 는 cis 와 trans 의 이성질체로 배향이 가능한데 일반적으로 trans 이성질체가 cis 이성질체보다 더 청색 이동(blue shift) 하는 것을 볼 수 있다. 또 1800 cm^{-1} 에서는 상대적으로 청색 이동의 위치인 1830 cm^{-1} 부근에서 나타나는 청 밴드와 그와 반대로 적색 이동의 위치인 1800 cm^{-1} 부근에서 나타나는 적 밴드 두 가지로 나타난다.1 차 구조 알킬 아질산염의 광반응 해리 과정에서 나타나는 이런 밴드들을 분석하고 이해함으로써 우리는 용액 상의 NO 의 방출과 재결합에 대해 연구할 수 있었다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-295**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Method for TEM detection of single-molecule protein dynamics

박상원 김성근[1,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

Transmission electron microscopy (TEM) is emerging as a powerful tool for soft matter studies. Because of the destructive nature of electron beam toward soft organic matter, TEM has found only limited use in biological studies. There are new techniques, however, that have been proposed to minimize the sample damage by using cryogenics or graphene liquid cell (GLC), the latter with an added advantage of observing real-time dynamics in the solution phase. Here, we propose a method to directly observe single-molecule protein dynamics in GLC by tagging sub-nanometer nanoparticles to the protein just as a protein is tagged by fluorophores in fluorescence microscopy. Unlike proteins that consist mostly of light elements, nano particles contain heavy elements that strongly scatter electron. By tagging two nanoparticles at specific sites of our interest, we can determine the distance between the particles and track protein motion along this coordinate. We expect that this technique is compatible and complementary to the FRET technique and even superior in the distance range below 1 nm and above 10 nm that is beyond the scope of FRET.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-296**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Single-molecule Study on Flexibility and Kinetics of Fab from Immunoglobulin G

박소영 오레나 김성근*

서울대학교 화학부

Immunoglobulin G (IgG) is a major type of antibody in blood that binds to the antigen and ultimately protects the immune system in the body. Two identical arms of Y-shaped IgG called Fab have binding regions for antigens at the end of the arms. It is assumed that the arms are flexible enough for versatile antigen recognition. Although a recent study using computer simulation and individual particle electron tomography showed a flexible and fluctuating IgG antibody particle, observing the interaction of the two arms in real time in solution remains a challenge. In this study, application of total internal reflection fluorescence and alternating-laser excitation techniques demonstrates the flexibility and reveals the kinetics of the Fab arms in real time. This technique does not require a multi-reference refinement process as other techniques often do, while providing reliable information about the kinetics of antibody under different conditions such as the presence of other antigens.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-297**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal-enhanced fluorescence properties of type-I and type-II quantum dots near nanoporous silver substrates

양원근 채원식*

한국기초과학지원연구원 대구센터

Recently, metal-enhanced fluorescence (MEF) behaviour attracts multidisciplinary researchers from basic to environmental sciences. Plasmonics from metal nanostructures reveals new physical insights because of interesting physical phenomena such as electromagnetic fields accumulation and radiative rate engineering. Fluorescent molecules near a plasmonic metal surface show unique emission properties, which are manifested by modulations in intensity, wavelength, and lifetime. In particular, nanostructured plasmonic metals enable remarkable amplification of the optical signals due to enhanced electromagnetic interactions between the adjacent fluorophores and metal surface. In this study, we investigated metal-enhanced fluorescence properties of quantum dots of different types, type-I and type II, using nanoporous silver membrane substrates. The observed fluorescence properties revealed that the emissions from the adjacent quantum dots were obviously affected by surrounding metal skeletons and the semiconductor types, which was clearly demonstrated by the well-established time-resolved fluorescence microscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-298**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Benchmark Studies of Density Functional Theory for Neutral Gold Clusters, Au_n(n=2−8)

백희현 문지원 김중한*

가톨릭대학교 화학과

Gold clusters have attracted much attention due to unique applications in nanoelectronics and catalysis industry. Because of the links between the structures of clusters and catalytic activity, identifying low-lying structures of the gold clusters is crucial. We present the high-level ab initio calculated results of neutral gold clusters, Au_n(n=2−8) using the coupled-cluster singles and doubles including the perturbative corrections for triple excitations (CCSD(T)). In addition, we report the results of benchmark studies of 44 density functional theory (DFT) methods for calculating structural and energetic parameters of Au_n(n=2−8). On the basis of the calculated results, RevTPSS demonstrates good performance for calculating the bond lengths and energetics, although it appears relatively moderate results for calculating bond angles. B3P86 performs well for calculating the vertical ionization potentials. We concluded that in small gold clusters system, at least quadruple-ζ level of basis set should be needed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-299**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Rebinding Dynamics of CO with Myoglobin at Low pH using Time-resolved vibrational spectroscopy

신주향 임만호*

부산대학교 화학과

Myoglobin (Mb) is one of the simplest heme proteins and has been studied extensively using a variety of physical techniques. The heme group in Mb is included in the protein matrix and covalently linked to the protein through the proximal histidine. The central iron atom reversibly binds ligands such as O_2 and CO at the sixth coordination site on the distal side of the heme. In this study, We measured the rebinding dynamics of the CO complex of Myoglobin at low pH using time-resolved vibrational spectroscopy. The stretching mode of ^{13}CO bound to the protein shows three stretching bands at 1920 cm^{-1}(A0), 1990 cm^{-1}(A1) and 1889 cm^{-1}(A3) . Ligand binding to Mb is a multiphasic process with fast geminate rebinding taking place on the nanosecond timescales and slower bimolecular rebinding occurring on microsecond timescales. The fast geminate rebinding of CO to Mb was from the distal histidine imidazole oriented out of the heme pocket, open conformations(A0). It suggests that according to conformations of protein affects rebinding kinetics of photolized CO.References[1] Wei Dong Tian; J. Thimothy Sage; Paul M. Champion, Probing Heme Protein Conformational Equilibration Rates with Kinetics Selection. Biochemistry 1996, 35, 3487-3502.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-300**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication, Characterization, and Applications of Inoxidizable Copper Nanoparticles

이용준 김경준 최은숙 신익수* 신권수*

숭실대학교 화학과

Abstract: Copper is one of the important metal catalyst and more specifically, its highly effective catalytic reaction on their surface is being applied in metal catalyst techniques. Unfortunately, copper can be easily oxidized at room temperature, which can be an obstacle to maintain its integrity in commercial areas. Herein, we describe the synthesis of inoxidizable copper nanoparticles (CuNPs) by using polyvinylpyrrolidone (PVP) during polyol fabrication process. In the method, copper sulfate and ascorbic acid were steadily dropped into the solution composed of PVP, sodium phosphate, and ethylene glycol mixture under the refluxing condition. The resulting CuNPs with PVP coating showed excellent resistance against oxidation and coagulation, and then they were employed as surface-enhanced Raman scattering (SERS) substrate and solid phase catalyst for the catalytic reduction of 4-nitrophenol to 4-aminophenol. Additionally, CuNPs were drop-casted on the working electrode, and applied to the electrocatalytic determination of nitrite.References K. S. Shin, Y. K. Cho, J. Y. Choi, K. Kim. Applied Catalysis A: General. 2012, 413-414, 170-175.K. Kim, H. S. Lee. J. Phys. Chem. B. 2005, 109, 18929-18934.P. H. Zhang, Y. M. Sui, G. J. Xiao, Y. N. Wang, C. Z. Wang, B. B. Liu, G. T. Zoua, B. Zou. J. Mater. Chem. A. 2013, 1, 1632-1638.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-301**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Displacement Processes and Domain Structure of Pre-adsorbed Triphenylphosphine on Au(111) by Decanethiols

한명수 노재근[1,*]

한양대학교 나노융합과학과 [1]한양대학교 화학과

Triphenylphosphine (TPP) is a specific capping agent that is produced from the synthesis of small size gold nanoparticles. For the decade, some scientists that have been interested in the plasmonics have synthesized the nanoparticles stabilized by this agent successfully and characterized their optical properties. But they knew the behavior of TPP as a capping agent on Au surfaces inexactly. Recently, scanning tunneling microscopy (STM) measurement clearly investigated the real surface behavior of TPP self-assembled monolayer (SAM) under ultra-high vacuum (UHV) condition. From these insights, the solution immersion of TPPs on Au(111) is conducted, because phosphine-stabilized AuNPs are controlled in solution phase not in UHV system. Using STM, the instability of TPP SAMs on Au(111) was confirmed with the displacement by 1-decanethiol (DT). As increasing the time of displacement, more dense DT domains with the striped pattern that is lying to the surface due to the toluene solvent covered the entire surface. And in the reverse scheme which the well-ordered DT SAMs were immersed in the TPP toluene solution there were not TPP layers on this Au substrate shown in the STM images. This observation was supported by the shift of cathodic potential of desorbed species in linear sweep technique of cyclic voltammetry. With these techniques, the process of structural evolution as a function of time of displacement could be more detectable. This result implied that the strong lateral interaction on the surface contributes to the stability of SAMs more than the affinity between Au and soft matter.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-302**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation and Structure of Alkaneselenocyanates Self-Assembled Monolayers on Au(111) Studied by Scanning Tunneling Microscopy

한슬기 노재근*

한양대학교 화학과

Self-assembled monolayers (SAMs) of thiols on metal surfaces have been frequently used for various practical applications such as biosensor, electronic devices and nanotechnology. In the present day, thio-sulfates, -chlorides, -cyanates and selenols are received much attention as other head groups instead of thiol due to oxidation problem of organosulfur during SAM formation. In this work, we prepared SAMs of alkaneselenocyanates of different alkyl chain length [butaneselenocyanate (C4Se-CN), octaneselenocyanate (C8Se-CN), and dodecaneselenocyanate (C12Se-CN)] on Au(111) from both solution and ambient-pressure vapor deposition method and characterized their SAMs by scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS). STM investigation shows that the formation and structure of alkaneselenocyanate SAMs on Au(111) were affected by alkyl chain length, temperature and deposition method. From C8SeCN SAMs formed at 363 K for 1 h from vapor deposition, we found that the SAMs have well-ordered domains with a (2 × 7) structure, while C12SeCN SAMs in 0.01 mM ethanol solution formed at 348 K for 2 h have well-ordered mixed domains with ($\sqrt{3} \times 7$) and ($\sqrt{3} \times \sqrt{3}$) packing structures. XPS study indicates that these alkaneselenocyanates SAMs were formed via chemical reaction between Se and gold surface result from RSe-CN bond cleavage by reduction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-303**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Growth Processes and Structures of 4-Fluorobenzenethiol and 4-Fluorobenzeneselenol Self-Assembled Monolayers on Au(111): head group effect

성시천 노재근*

한양대학교 화학과

Self-assembled monolayers (SAMs) are ultrathin film of organic molecules which are usually consisted of head group, alkyl or aromatic spacer and terminal group. All the structural components play crucial role in determining specific characters of SAMs. SAMs invest surface of their substrate with special electrical and physical property. Especially, SAMs having aromatic backbone structure with fluorine substituent are useful in molecular electronics because of their ability to modify work function of metal surface. Since energy barrier of surface is significantly affected by density and orientation of adsorbed organic molecules, it is important to illuminate the packing structure of SAMs. Focusing on this issue, we have compared two different head groups, sulfur and selenium. The SAMs were prepared from 4-fluorobenzene thiol (4-FBT) and 4-fluorobenzeneselenol (4-FBSe), and characterized by scanning tunneling microscopy (STM) and cyclic voltammetry (CV) to investigate structure and electrochemical behavior of the SAMs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-304**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation and Nanostructure of Self-Assembled Monolayers on Au(111) by Adsorption of Unsymmetric Adamantyl Hexyl Disulfide

손영지 한슬기 노재근*

한양대학교 화학과

Self-assembled monolayers (SAMs) formed by the adsorption of organic molecules containing sulfur headgroup on metal surfaces are simple and flexible systems to control the physical and chemical properties of solid surfaces. In paticular, symmetric or unsymmetric dialkyl dislufides have been often used for understanding the formation and strcuture of SAMs and for the fabrication of molecular thin filmes in nano and biotechnology. However, there are no reports describing the formation and strcuture of SAMs on Au(111) derived from unsymmetric adamantyl hexyl disulfide (AHDS): the admantyl group has aliphatic cage strcuture, while the hexyl group has normal alkyl chain. Molecular-scale scanning tunneling microscopy revealed the unique ordered domains of AHDS SAMs on Au(111), which have never been observed from those observed from single component adamantanethiol SAMs or hexanethiol SAMs. In this presentation, the formation and strcuture of AHDS SAMs on Au(111) will be discussed in more detail.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-305**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fullerene-like MoC nanocrystals for Electrocatalytic Hydrogen Evolution Reaction

권익선 박정희[1,*]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과

Hydrogen energy is an ideal, clean and efficient secondary energy resource. Noble metals such as platinum and palladium are well-known for their superior electrocatalytic property in the hydrogen evolution reation (HER) in an acidic medium and commonly used as electrocatalysts in the applications. However, large-scale application of them is limited due to their high prices and global low availabilities. Therefore, extensive research efforts have been devoted to the development of non-platinum electrocatalysts for HER. Here, we show the synthesis of fullerene-like (FL) MoC nanocrystals and their excellent electrocatalytic activity. We achieved this by a pulsed laser induced liquid–solid interfacial reaction. With the merits of the defect-induced additional active edge sites, the defect-rich FL MoC nanocrystals exhibit excellent HER activity, which demonstrates the best integrated electrocatalytic performance. Finally, This study successfully demonstrates that introducing strain to FL MoC is feasible by wavelength tuning of Nd:YAG pulse laser. Introducing vacancies and strain may open up a potential pathway for designing more efficient Mo-based catalyst for HER.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-306**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optical properties of strained ZnSe and CdSe nanowires

김예진 임형순[1] 박기동[1] 김준동[2] 박정희[*]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자 [2]고려대학교 세종캠퍼스 소재화학과

For the fabrication of integrated semiconductor nanowire devices, the correlation between the optical properties and mechanical strength needs to be carefully examined. We investigated the dependence of the optical properties of strained ZnSe and CdSe nanowires (NWs) on their crystallographic structure. ZnSe and CdSe NWs with a controlled growth direction were synthesized using the vapor transport method. Zinc blende (ZB)-wurztite (WZ) polytypic structures was successfully produced using the growth condition. The use of Ni nanoparticle catalysts induced the ZB phase [011] growth direction for both ZnSe and CdSe NWs. The NWs were bent by the mechanical buckling of poly(dimethylsilioxane), which transformed the initially straight NWs into wavy shapes via releasing of the pre-strains. Micro-photoluminescence (PL) spectra were collected for individual NWs under various bending strains (

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-307**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A step forward into enhanced stability of CsPbI$_3$ by introducing Cl/Br

서재민 박정희* 김준동[1] 임형순[2] 박기동[2] 임영록 김영운[3] 박정원[4] 손창용 차승환[5] 권익선[2] 곽인혜[2] 김덕환 김도연

고려대학교 소재화학과 [1]고려대학교 세종캠퍼스 소재화학과 [2]고려대학교 미세소자공학협동/마이크로소자 [3]호서대학교 그린에너지공학과 [4]고려대학교 미세소자공학협동과정 [5]호서대학교 그린에너지융합과

Cesium lead iodide is a semiconductor that possesses an excellent combination of band gap and absorption coefficient for photovoltaic applications in its perovskite phase. However, It is well known that it does not preserve its equilibrium structure under ambient conditions; upon formation at room temperature it exhibits a yellow orthorhombic phase with wide bandgap, unsuitable for solar cell applications. Here we demonstrate Chem. Vapor Deposition (CVD) growth of CsPbI$_3$ nanowires maintain black cubic phase at room temperature. Nevertheless, the resulting cubic phase CsPbI$_3$ nanowires turns to be yellow in few days as well. In order to achieve improved stability of functional perovskite phase, we controlled the ratio of precursors, particularly at levels near the limit for chloride (or bromide) in a cesium lead iodide host.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-308**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal Nanoparticle Embedded on Nitrogen-doped Graphitized Nanodiamond as Electrocatalyst

박정원 박정희[1,*] 권익선[2] 손창용[1] 김예진[1] 박기동[2] 임형순[2]

고려대학교 미세소자공학협동과정 [1]고려대학교 소재화학과 [2]고려대학교 미세소자공학협동/마이크로소자

A low-cost and highly efficient electrocatalyst to replace Pt-based catalysts for hydrogen evolution reaction (HER) has attracted increasing interest in renewable energy research. Here, we report that metal nanoparticles (Au, Ag) embedded on the N-doped graphitized nanodiamonds (metal-NGNDs) have an effect on hydrogen evolution reaction. The NDs, transformed into the graphitized onion-like form by laser-induced reaction, were doped with the N atoms by the thermal annealing under NH_3 gas. The efficient performance is credited to the pyrrolic-like N electronic structures of NGND that combined with the active metal nanoparticles. The metal-NGND nanostructures exhibits low overpotential and selectivity for hydrogen evolution reaction. This finding may lead to a new strategy to develop cost-effective electrocatalysts with superior efficiency for another electrocatalytic reactions such as CO_2 reduction reaction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-309**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Niobium phosphide nanowires for efficient electrocatalytic hydrogen evolution reaction

손창용 박정희* 김덕환 김예진 박정원[1] 서재민 김영운[2]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동과정 [2]호서대학교 그린에너지공학과

Production of molecular hydrogen by the electrochemical reduction of water is an important component of several developing clean-energy technologies. The hydrogen evolution reaction constitutes half of the water-splitting reaction. Currently, platinum is the best known hydrogen evolution catalyst with only small overpotentials and high reaction rates, but the scarcity and high cost may limit its widespread technological use. Recently, transition metal phosphides, including Ni_2P, CoP, and FeP, have been identified as promising hydrogen evolution reaction electrocatalysts. Herein, we synthesized Niobium phosphide nanowire arrays using a unique gas-phase anion exchange reaction of pre-grown Nb_2O<sub)5 nanowires with phosphine gas. This method provides many benefits including no extra fabrication process, high yield, short reaction time, and excellent reproducibility. Their electrocatalytic performance was tested for hydrogen evolution reaction, showing an excellent catalytic activity and stability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-310**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photodetection of $(GaAs)_{1-x}(Ga_2Se_3)_x$ Alloy Nanowires

박기동 김준동[1] 임형순 김예진[2] 박정희[2,*]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 세종캠퍼스 소재화학과 [2]고려대학교 소재화학과

Multicomponent nanowires are of great interest for integrated nanoscale optoelectronic devices owing to their widely tunable band gaps. In this study, we synthesize $(GaAs)_{1-x}(Ga_2Se_3)_x$ ternary composition alloy nanowires using the vapor transport method. The formation of a cubic (zinc blende) phase solid solution at the composition range of $x = 0\text{-}0.5$ allowed the tuning of the band gap (1.4–2.0 eV). Pure GaAs NWs were synthesized with a controlled growth direction; [111] and [112], using a hydrogen gas flow during the growth. As the Ga_2Se_3 incorporated during the growth under H_2 flow, the NW becomes defect-free single-crystalline and their growth direction is converted homogeneously into [110]. The Ga vacancies of Ga_2Se_3 along the [110] direction may also contribute to produce the uniform growth direction of NW. The incorporation of Se into the GaAs nanowires induces higher photo-sensitivity and lower dark current, which opens up a new strategy for enhancing the performance of photodetectors.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-311**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

IrO_2-ZnO and RuO_2-ZnO hybrid nanoparticles as highly efficient bifunctional electrocatalysts

곽인혜 박정희[1,*] 임형순 임영록[1] 박기동

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과

The fabrication and design of earth-abundant and high-performance catalysts for the bifunctional oxygen evolution and reduction (OER and ORR) are very crucial for the development and commercialization of sustainable energy conversion technologies such as metal-air batteries. The bifunctional oxygen catalysts could produce extremely high energy density of metal-air batteries. To date, the most efficient electrochemical OER catalysts are known to be ruthenium (RuO_2) and iridium oxides (IrO_2), despite their limited availability and high cost. In the present work, we report the high electrocatalytic OER and ORR activities of 10 % RuO_2- and IrO_2-ZnO hybrid nanocrystals (NCs), which are comparable to pure RuO_2 or IrO_2. In this way, the cost problem will be improved, using a cheap and earth abundant ZnO support. The excellent electrocatalytic activity was rationalized by a synergistic effect in which ZnO nanocrystal matrix effectively guards the active RuO_2 or IrO_2 nanocrystals that distributes homogeneously with a 1-2 nm size.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-312**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Zn_2GeO_4 and Zn_2SnO_4 Nanowires for High-Capacity Lithium- and Sodium-Ion Batteries

임영록 임형순[1] 박기동[1] 박정희*

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Germanium (Ge) and Tin (Sn) are considered to be the most promising alternatives to commercial carbon materials in lithium- (LIBs) and sodium-ion batteries (SIBs). High-purity zinc germanium oxide (Zn_2GeO_4) and zinc tin oxide (Zn_2SnO_4) nanowires (NWs) were synthesized using a hydrothermal method, and their electrochemical properties as anode materials in LIBs and SIBs were comparatively investigated. The NWs had a uniform morphology and consisted of single-crystalline rhombohedral (Zn_2GeO_4) and cubic (Zn_2SnO_4) phases. For LIBs, Zn_2GeO_4 and Zn_2SnO_4 NWs showed an excellent cycling performance, with a reversible capacity of 1022 and 692 mA h g-1 after 50 cycles, respectively. Their high capacities are attributed to a combination of a reversible conversion reaction of Zn_2GeO_4 (or Zn_2SnO_4) and an alloying reaction of Ge (or Sn) and Zn. For the first time, we examined the cycling performance of Zn_2GeO_4 and Zn_2SnO_4 NWs in SIBs; their maximum capacities were 357 mA h g-1 and 337 mA h g-1 after 50 cycles, respectively. Zn_2GeO_4 NWs exhibit a much higher capacity than the theoretical capacity (100 mA h g-1), probably due to a favorable alloying reaction for the amorphous Ge. The capacity of Zn_2SnO_4 suggests there is a kinetic difficulty for the Na–Sn alloying reaction to reach the theoretical composition (Na3.75Sn), although the reversible conversion reaction contributes in increasing the capacities. The present systematic comparison between the lithiation and sodiation will provide valuable information for the development of high-performance LIBs and SIBs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-313**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tantalum Oxinitride Photocatalysts for Enhanced Solar-Driven Photoelectrochemical Water Splitting

김영운 박정희[1,*] 차은희[2,*] 차승환[3] 손창용[1] 김덕환[1]

호서대학교 그린에너지공학과 [1]고려대학교 소재화학과 [2]호서대학교 제약공학과 [3]호서대학교 그린에너지융합과

The solar-driven photoelectrochemical splitting of water offers an attractive means of generating hydrogen fuel, which is free from environmental issues related to the combustion of fossil fuels. Tantalum oxynitride (TaON) is an n-type semiconductor, and has received recently increasing attention as a photoanode for solar water splitting. Because of a band gap of about 2.5 eV with suitable energy positions, TaON can utilize a large portion of the solar spectrum (< 500 nm). Herein, we developed unique synthesis method for high-yield TaON nanoparticles by combining a sol-gel method and a gas phase substitution reaction. In order to improve the efficiency and stability, we used a strategy, doping or substitution of other elements, and their much better performance than that of TaON for solar-driven PEC water splitting. The elemental substitution shifts cathodically the flat band potential, and simultaneously enhance the water oxidation which suppresses effectively the oxidation of TaON.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-314**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of transition metal dichalcogenides(NiSe2,CoSe2) with CVD method

차승환 차은희[1,*] 박정희[2] 김영운[3]

호서대학교 그린에너지융합과 [1]호서대학교 제약공학과 [2]고려대학교 소재화학과 [3]호서대학교 그린에너지공학과

As typical members of transition metal dichalcogenides, such as nickel diselenides & cobal diselenides, exhibit interesting electronic and magnetic properties, and have found several applications in the fields of conductivity, catalyst, optical recording materials, solar cells, lithium ion cells, sensors, laser materials and optical fibers.In this purpose, synthesis of transition metal dichalcogenides comprises two steps.First, transition metal film is deposited on the silicon wafer by dipping process. Second, dichalcogenides were synthesized using Selenium powder with tube furnace.In this communication, we have demonstrated the synthesis of transition metal dichalcogenides crystals via a CVD with tube furnace route, an emerging efficient earthabundant catalyst that was reported recently

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-315**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Ultrasound Synthesis of Composition- and Size-Controlled Lead Halide Perovskite Nanocrystals

김덕환 박정희* 김영운[1]

고려대학교 소재화학과 [1]호서대학교 그린에너지공학과

Lead halide perovskites have attracted enormous interest as excellent light absorber material in photovoltaics with the power conversion efficiency exceeding 20%. Synthesis of colloidal perovskite nanocrystals (NCs) is challenging because of their outstanding optical properties such as high quantum yield emission. Herein, we report a novel ultrasound-induced synthesis method that can be applicable for wide-range composition $APbX_3$ perovskite, where A = CH_3NH_3 or Cs, $HN{=}CHNH_3$ (formamidinium), and X = Cl or Br, I, with a controlled quantum dot size (2-10 nm). Ultrasonic irradiation accelerates the dissolution of precursors in toluene, which determines the growth rate of NCs. The size reduction to 2 nm increases significantly the band gap, possibly due to the 2-dimemisional quantum confinement effects. We fabricated high-sensitivity photodetectors by spin coating the perovskite NCs homogenously on a large-area silicon oxide substrates, showing a great potential to fabricate optoelectronic devices.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-316**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

TEM-NED법을 이용한 NCM 전극재료의 Li 이동에 따른 격자변형 및 상변화 연구

김준동 박정희[1,*] 안재평[2,*]

고려대학교 세종캠퍼스 소재화학과 [1]고려대학교 소재화학과 [2]한국과학기술연구원(KIST) 산업화지원센터

NCM 으로 불리는 Li(NiCoMn)O2 은 차기 리튬 이온 배터리 분야에서 가장 중요한 양극물질이다. 기존의 리튬 이온 배터리 물질에서 쓰이고 있는 LiCoO2 와 비교하여 더 높은 용량과 값싼 비용으로 인하여 각광을 받고 있다. 그러나 높은 전압에서 작동 시 NCM 의 경우 충·방전을 반복함에 따라서 급격하게 용량이 감소하는 현상이 발생한다. 이러한 열화현상은 양극재료의 구조가 변형되거나 붕괴되기 때문으로 알려져 있지만 Li 의 입출입에 대해 지금까지 직접적으로 규명한 사례는 극히 제한적이다. 본 연구에서는 투과전자현미경에서 나노회절패턴과 전자빔의 세차회절 방법을 동시에 사용하여 상변화 또는 격자변형을 측정함으로써 NCM 의 열화 원리를 연구하였다. 측정 및 해석을 위해 상변형에 대해 ASTAR 와 격자변형에 대해 Top Spin 을 사용하였다. 이 방법은 2 nm 의 매우 작은 영역만을 회절시킴으로 양극입자의 어떤 부위라도 국부적인 나노회절패턴을 얻고 해석할 수 있다. 또한 2 nm 이하의 전자빔을 스캔하여 특정 면적에 대해 10~20 만장 정도의 나노회절패턴을 매트릭스 형태로 측정하여 분석하기 때문에 기존의 HRTEM 이미지와 SAD 패턴의 단점이었던 해석의 모호성을 제거할 수 있는 장점을 갖고 있다. 본 연구에서는 최근 모바일 이차전지의 중심이 되고 있는 NCM 양극재료에서 Li 의 충·방전 동안에 발생하는 양극재료의 격자변형과 상변태 현상을 지금까지와는 전혀 다른 방법으로 추적하였다. 이를 통해 NCM 의 위치에 따라 격자 변형량을 측정하여 상변화에 필요한 격자의 임계 변형량을 측정하였으며 더욱이 변형량으로 NCM 내에 Li 잔존량을 계산할 수 있었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-317**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Metal monochalcogenide and their characterization

김도연 박정희* 박기동[1] 임형순[1]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자

Recently, Many groups pay attention to 2D materials and their fascinating properties.We successfully synthesized one kind of metal-monochalcongenide monolayer GaSe.Gallium selenide (GaSe) is a typical layered metal monochalcogenide, which has a indirect/direct bandgap of 2.0 eV, and shows p-type semiconductor behavior. Hexagonal/rhombohedral phase GaSe has unique Se-Ga-Ga-Se layered repeating unit built by six-membered Ga3Se3 rings and adjacent layers are held together by van der Waals interactions. This GaSe monolayer is expect to next-generation flexible electronic and optoelectronic devices such as photodetectors and field-effect transistors. Herein, we synthesized GaSe monolayer via chemical vapor deposition method. The size, shape, and thickness of the GaSe monolayer were controllable by growth duration, growth temperature, and gas flow rate. Large-area and single-crystalline GaSe monolayers were successfully synthesized with a thickness of 0.8 nm and a width of 10~20 μm.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-318**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Polytype GaP and GaAs Nanowires and their Bending Deformation

임형순 박정희[1,*] 박기동 김준동[2]

고려대학교 미세소자공학협동/마이크로소자 [1]고려대학교 소재화학과 [2]고려대학교 세종캠퍼스 소재화학과

The mechanical properies of GaP and GaAs nanowires (NWs) were investigated using Raman spectroscopy. Two different growth directions, [111] and [112], was controlled without changing the diameter (150 nm); the H2 flow during growth induces the the [112] direction. The GaP NWs consisted of twinned superlattice structures domains which is perpendicular or parallel to the growth direction. Remarkably, the bending deformation of GaP [112] NWs is larger than that of the GaP [111] NWs, probably due to the shorter period of the twin domains. On the other hand, the GaAs NWs have a negligible amount of superlattice domains, compared to the GaP NWs. The bending deformation occurs more significantly for the GaP NW than the GaAs NW, indicating the stacking faults along the growth direction plays an important role in increasing the bending deformation. These results suggest that the more stacking faults produces the higher strain of the NWs.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-319**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of nearly monodisperse Fe3O4 and Fe@Fe3O4 nanoparticles coated with various biocompatible ligands and silica

tirusew tegafaw 이강호*

경북대학교 화학과

Iron-based nanoparticles are extremely valuable for biomedical applications because of their large magnetization values at room temperature and low toxicity. In this study, we synthesized nearly monodisperse Fe3O4 and Fe@Fe3O4 (core: Fe, shell: Fe3O4) nanoparticles in aqueous phase under argon flow, and coated them with various biocompatible ligands and silica. We characterized the prepared surface-modified nanoparticles using HRTEM, XRD, FT-IR, SQUID, XPS, PL, confocal microscopy, and cytotoxicity. The results show that the surface-modified nanoparticles are biocompatible and potential candidates for various biomedical applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-320**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrostatic charge distribution in neutral Ag-Au alloy clusters

임은학 허지영[1] 김성근[*]

서울대학교 화학부 [1]상명대학교 의생명공학과

Silver and gold form one of the most widely used metal alloys. Both elements have nearly identical characteristics including valance electron configuration ($d^{10}s^{1}$) and lattice constant (Ag: 4.0853 Å, Au: 4.0782 Å), which allow them to be fully miscible over a wide range of length scales from clusters to the bulk phase. In this study, we carried out density functional theory calculations for the geometrical and electronic structures of the Ag-Au alloy clusters, which inadvertently revealed some generic regularities in their electrostatic charge distributions. We propose a set of "rules" to explain them and even predict the charge distributions in the unknown Ag-Au alloy clusters or bulk solids.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-321**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Comparison Study on the Binding Affinity between Stapled p53/MDM2 and cHLH/MDM2

임해리 여진희 함시현*

숙명여자대학교 화학과

The p53 tumor suppressor protein loses its activity upon binding with MDM2 protein, and inhibition of the interaction between p53 and MDM2 is significant to activate the function of the p53 protein. Recently, the stapled p53 protein and the cyclized helix-loop-helix peptide (cHLH) mimicking the α-helix part of p53 protein has been designed and found to exhibit high binding affinity with MDM2. Here, we report the structural and thermodynamic characteristics for the binding complex of the stapled p53/MDM2 and cHLH/MDM2. We performed molecular dynamics simulations to investigate the structural properties of the two complexes. The binding free energy calculation based on the integral equation theory was also executed to quantify the binding affinity for the two complexes and to understand the factors responsible for the binding affinity. Additionally, we compared the binding affinity between the stapled p53/MDM2 and cHLH/MDM2, in order to find the more suitable inhibitor of the p53/MDM2 complex.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-322**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

New and Efficient Noble Metal Free Copper Molybdenum Sulfide (Cu2MoS4) Nanosheet as Co-catalyst for Excellent Photocatalytic Hydrogen Evolution Reaction(HER) via Water Splitting

홍상엽 DHARANI PRAVEEN KUMAR[1] devulapalliamaranathareddy 최지하 김태규*

부산대학교 화학과 [1]POSTECH 화학과

The charge carrier recombination and durability issues are major problems to take in photocatalytic hydrogen (H2) evolution process. Thus, it is an urgent need to develop an efficient photocatalyst to controlling charge-carrier dynamics in the photocatalytic system. Herein we developed copper molybdenum sulfide (Cu2MoS4) nanosheets cocatalysed CdS nanorods to control charge carriers without recombination and utilization of photocatalytic H2 evolution under simulated solar light irradiation. This effective control and utilization of charge carriers is due to the loading of Cu2MoS4 nanosheets on CdS nanorods, it compensate the restrictions of CdS and stimulates a synergistic effects such as efficient photoexcited charge separation and improved photo stability with its layered structure. This layered Cu2MoS4 nanosheets have emerged as novel and active replacement for the precious noble metals as a co-catalyst for photocatalytic H2 production by water splitting. The rate of H2 production exhibited superior activity through evidence of Cu2MoS4 on CdS nanoparticles. The physicochemical properties were analyzed by various characterization techniques.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-323**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

RGO/BiOI/AgI nanocomposite advanced the photocatalytic activity under solar light irradiation

ISLAMMOHAMMADJAHURUL devulapalliamaranathareddy 마로리 김유진 김태규*

부산대학교 화학과

Nanocomposite based photocatalysts are used for solar energy harvesting and utilizing through in situ interfacial charge separation and low efficiency is the vital problems. To improve the interfacial charge transfer efficiency, herein we were successfully fabricated three dimensional bismuth oxyiodide based RGO/BiOI/AgI nanocomposite in ethylene glycol and water solvents through a simple precipitation method. The photocatalytic performance of the as-synthesized nanocomposites was carried out for the degradation of rhodamine B (RhB). RGO has prolonged the photocatalytic activity of the RGO/BiOI/AgI nanocomposites under simulated solar light irradiation by the effective interfacial charge carrier's separation and efficient interaction between RGO and RhB molecules. In addition, the ease of separation of the three dimensional RGO/BiOI/AgI nanocomposite exhibited a higher order of reusability and long term photocatalytic stability.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-324**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The study on the origin of PDMS properties changes according to the mixing ratio

조한샘 문혜영[1] 이홍순[2] 정세채[3,*]

한국표준과학연구원(KRISS) 미래측정기술부/의료융합측정표준센터/ [1]가천대학교 글로벌캠퍼스 바이오 나노대학/나노화학과 [2]한국표준과학연구원 미래융합기술부 의료융합측정표준센터 [3]한국표준과학연구원(KRISS) 양자연구부 분광그룹

Polydimethylsiloxane(PDMS)는 생체조직과의 유사성 및 생물 안정성이 뛰어난 특성을 갖기 때문에, 생물의학적 분야에서 다양하게 응용기술이 개발되고 있다. 최근 연구에 따르면 pre-polymer 와 cross-linker 의 배합비율에 따라서 PDMS 의 기계적 특성뿐만 아니라 물리적, 광학적, 표면적 성질을 제어할 수 있다고 알려져 있다. 하지만 PDMS 의 이러한 특성들이 어디에서 기인하는지에 대한 원인은 아직 규명되어 있지 않다. 본 연구에서는, Dow corning 사의 SYLGARD184 pre-polymer 와 cross-linker 의 배합 비율(1:1, 1.5:1, 2:1, 3:1, 5:1, 7:1, 9:1, 10:1, 12:1, 20:1, 30:1)에 따른 PDMS 의 기계적, 물리적, 광학적, 표면 특성들을 다면적, 통합적으로 분석하고자 하였다. 이를 위하여, PDMS 의 Young's modulus, 밀도, 굴절률, 접촉각 및 표면 거칠기를 배합비율에 따라 측정을 하였다. 배합비율이 9:1 인 경우에 Young's modulus, 밀도, 굴절률, 접촉각이 최대 혹은 최소값을 갖는 것을 확인할 수 있었다. 라만 및 흡수분광기술을 활용하여 각각의 배합비율의 PDMS 의 cross-linker 를 구성하는 기능기인 Si-H 결합과 pre-polymer 에 있는 C=C 결합의 정량적 측정 방법을 제안 및 적용하였다. 이를 통하여 PDMS 의 cross-linking 반응에 사용된 Si-H 및 C=C 의 양을 결정할 수 있었으며, 각각의 배합비율에 따른 생성된 단위 부피당 cross-linked network 의 양의 변화를 유추할 수 있었다. 이로부터 배합비율에 따른 PDMS 의 탄성계수의 변화는, 고분자 내 cross-linked network 의 volume fraction 의 탄성계수 의존성에 대한 molecular theoretical 예측과 동일함을 실험적으로 증명하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-325**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ultrafast Chemical Exchange Dynamics in Electrolyte of Lithium Ion Battery

박광희 이경구[1] 곽경원[*] 조민행[*]

고려대학교 화학과 [1]군산대학교 화학과

리튬이온 배터리에서 전해질은 리튬염을 carbonate 와 같은 유기용매에 녹인 용액을 사용하며 전해질 용액에 녹아 있는 리튬이온이 용액을 통해 이동하면서 충전이나 방전 과정이 진행된다. 우리는 리튬이온 배터리에서 사용하는 유기용매 중 하나인 Diethylcarbonate 에 $LiPF_6$ 를 녹인 용액을 2 차원 적외선 분광법(2DIR)으로 측정하고 carbonate 의 C=O 진동 스펙트럼을 관찰하고 이에 대한 peak volume 을 분석하여 매우 빠른 시간에서 발생하는 carbonate 용매와 리튬 이온의 chemical exchange 를 실험적으로 확인하였다. 이는 전해질 유기용매의 1 차 solvation shell 에서 발생하는 리튬이온은 매우 빠른 진입이나 탈출에 대한 증거라고 할 수 있다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-326**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electronic spectroscopy of jet-cooled indole-3-acetic acid in the gas phase and ab initio calculations

성연국 민아름 안아름 문철주 최명룡*

경상대학교 화학과

Indole-3-acetic acid (IAA) is the most common plant hormone that plays an essential role in the regulation of plant growth and fruit development. The special role in nature has led us to investigate the intrinsic properties of IAA in the gas phase. We have measured the electronic spectra of IAA by employing a resonant two-photon ionization (R2PI) technique in the free jet conditions. The mass-selective R2PI spectrum of IAA was measured in the spectral range of 34000-36000 cm^{-1}. In this work, the 0-0 band of the IAA monomer was observed at 35053 cm^{-1}. The vibronic assignment of the recorded R2PI spectrum of IAA will be presented. We also calculated the optimized structures of IAA by density functional theory (DFT) with a 6-311++G** basis set. Further investigation on the conformational information of IAA by using UV-UV hole-burning spectroscopic studies will be discussed in this presentation.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-327**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of oxygen-containing heterocyclic compound

강도원 김홍래* 권찬호*

강원대학교 화학과

We recorded the vibrational spectra of oxetane and tetrahydropyran cation in the electronic ground state by using the vacuum ultraviolet mass-analyzed threshold ionization technique (VUV-MATI). The adiabatic ionization energy of oxetane and tetrahydropyran was determined to be 77976 ± 5 cm^{-1} (9.6678 ± 0.0006 eV) and 74681 cm^{-1} (9.2583 ± 0.0006 eV), respectively. Based on well reproduced Franck-Condon fitting simulation, the vibrational assignment of peaks observed in the VUV-MATI spectra of oxetane and tetrahydropyran was performed and the cationic structure of oxetane and tetrahydropyran in the electronic ground state was determined.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-328**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Vibrational spectrum of mixture-crotonaldehyde cation by vacuum ultraviolet mass-analyzed threshold ionization spectroscopy

박성만 김홍래 권찬호*

강원대학교 화학과

We measured the vibrational spectrum of cationic state utilizing the one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy of mixture-crotonaldehyde. The vacuum ultraviolet generated by four-wave difference frequency mixing in Kr gas. The measured stereo-isomer specific VUV-MATI spectrum and analyzed through Franck-Condon simulations using the neutral and cationic geometries for trans-s-trans, trans-s-cis, cis-s-trans, cis-s-cis isomers of crotonaldehyde obtained at CAM-B3LYP/aug-cc-pVDZ level. The adiabatic ionization energy of trans-s-trans isomers determined to be 9.7051 ± 0.0007 eV, in excellent agreement with previously reported value, 9.75 eV. From the VUV-MATI spectrum and Franck-Condon simulations, we found the four origin band of stereo-isomer.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-329**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ionization energies and cationic structures of heterocyclic molecules and aldehydes by vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy

이유란 김홍래 권찬호*

강원대학교 화학과

We have constructed the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectrometer providing the VUV-MATI spectrum with a decent quality for the study on complicate vibrational structure of molecular cation. The key idea on construction of the VUV-MATI spectrometer with high-performance was originated from the basic concepts that very low PFI voltage is needed to improve the spectral resolution in the VUV-MATI spectrum and the dual stage extraction to achieve the first-order focusing of the MATI ions generated initially with the spatial distribution. Such an idea on instrumentation was rationalized by utilizing the SIMION program which is used to calculate the electric fields and the trajectories of charged particles for a unique configuration of the electrodes with voltage. Excellent performance of the constructed VUV-MATI spectrometer has been proved elucidating the complicated vibrational structure of pyridine cation. We expanded to determine the accurate ionization energies and conformational structure of saturated heterocyclic molecules and aldehydes which play an important role in biological system and conformational dynamics. Accurate ionization energies were determined from the measured the VUV-PIE curve and the VUV-MATI spectra. Vibrational assignments of the observed VUV-MATI spectra could be achieved utilizing the Franck-Condon factors and vibrational frequencies calculated by adjusting the geometrical parameters of cationic conformers at the B3LYP/cc-pVTZ level.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-330**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Adsorption behavior and characterization according to the various pH conditions of aminocyanobiphenyl derivatives (44ACBP and 3AB4CN) on silver surfaces: SERS and DFT study

엄소영 김홍래 권찬호*

강원대학교 화학과

Adsorption behavior of 3’-aminobiphenyl-4-carbonitrile (3AB4CN) and 4-amino-4’-cyanobiphenyl (44ACBP) on silver surfaces was investigated utilizing the surface-enhanced Raman scattering (SERS) which is well-established as a powerful spectroscopic tool for characterizing the adsorbates on metal surface. The SERS spectra of 3AB4CN and 44ACBP on Ag surfaces were measured in various pH conditions and the ordinary Raman spectra of neat sample in solid state were also taken for comparison with SERS spectra. Spectral assignments of the measured Raman spectra could be effectively achieved with an aid of density functional theory (DFT) calculation. In SERS spectra, the up-shifted and the broadening of the CN stretching vibrational peak indicate that the adsorption takes pace via CN bond on metal surface. In addition, the broadening for the -NH_2 rocking vibrational peaks indicates to be pseudo-parallel orientation of the two phenyl rings to the surface with the interaction of the -NH_2 group. Thereafter, the change of the pH to the acidic condition induced the appearance of the C-H stretching bands and the disappearance of the –NH_2 rocking vibrational peaks, which would rather be vertical orientation to silver surface. In the present work, it is worth noting that the molecular orientation against Ag surface could be reversibly controlled by the pH condition.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-331**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synergistic effects of ultrathin MoS_2 nanosheets on CdS nanorods for spectacular hydrogen evolution under solar light irradiation

DHARANI PRAVEEN KUMAR 홍상엽[1] devulapalliamaranathareddy[1] 김태규[1,*]

POSTECH 화학과 [1]부산대학교 화학과

Increasing global energy demand and concern for environmental safety have prompted research into abundant, environmental benign and sustainable energy alternative to fossil fuels. Solar energy is globally abundant; therefore, we focused on the effective utilization of solar energy to produce hydrogen gas via photocatalytic water splitting. Hydrogen has a high energy density and reacts with oxygen in fuel cells to produce electricity; in addition, only water is released during combustion, thereby eliminating the emission of polluting gases. The existing technology for photocatalytic water splitting primarily involves the use of noble metals, such as Pt, as cocatalysts on semiconductor materials resulting in significantly improved photocatalytic H_2 production. However, because of the high cost and low abundance of Pt, its practical use is limited. In this study, Noble-metal-free ultrathin MoS2 nanosheets-decorated CdS nanorods exhibited remarkably high rate of H_2 production of up to 174 mmol h^{-1} g^{-1} under natural solar light irradiation, showing one of the most excellent values ever reported on CdS/MoS_2 composites. The extraordinary active edge sites of ultra thin nanosheets of MoS_2 effectively separate the photogenerated charge carriers and improve the surface shuttling properties for efficient H_2 production. The structural, morphological and optical properties and its correlativity towards elevated hydrogen production will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-332**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mixed Metal Phosphides Derived from Layered Double Hydroxide Double-Shelled Nanocages as an Efficient Non-precious Co-catalyst for Hydrogen Production through water splitting

devulapalliamaranathareddy 김유진 이승희 최지하 **ISLAMMOHAMMADJAHURUL DHARANI PRAVEEN KUMAR**[1] 김태규*

부산대학교 화학과 [1]POSTECH 화학과

Non-precious transition metal phosphides (TMPs) are emerging as the most promising substitutes for expensive noble metal-based co-catalysts for the hydrogen evolution reaction. While the synthesis of TMPs is well established, it is extremely challenging to design porous multicomponent transition metal phosphides (MCTMPs) to overcome the drawbacks of TMPs, namely, limited active sites and low surface area. Herein, we synthesized MCTMPs (containing Co, Ni, and Mo) from layered double hydroxide double-shelled nanocages by a metal-organic framework (MOF) template-engaged strategy. Benefiting from the rich structural features, high specific surface area, and active multicomponents in the composition, the MCTMPs manifest greatly enhanced photocatalytic hydrogen evolution properties when integrated with CdS semiconductor nanorods. The observed hydrogen evolution rate is 53.76 fold higher than that of the bare CdS nanostructures and 4.37 times higher than that for the benchmark 2 wt% Pt–CdS nanorods, with a quantum efficiency of 40.6%. A possible explanation for the enhancement of the photocatalytic activity was proposed on the basis of the separation efficiency of the photogenerated charge carriers; this was further confirmed by photocurrent, electrochemical impedance spectroscopy, and photoluminescence studies. We believe that the work presented here represents a novel design strategy for MCTMPs with active noble metal free components with applications as sunlight-driven photocatalysts for hydrogen production through water splitting.Keywords: Mixed Metal Phosphides, CdS nanorods, Photocatalytic hydrogen, water splitting.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-333**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photophysical Investigation of meso-substituted porphyrins with symmetric arrangements in Neutral and Diacid Form

이예진 심상덕*

순천대학교 화학과

대칭적인 Meso-subsituted porphyrin 인 FFFF (tetrakis(pentafluorophenyl)porphyrin), AAAA (tetrakis(p-aminophenyl)porphyrin), MMMM (tetrakis-(mesityl)porphyrin), TPP (tetrakis(phenyl)porphyrin)의 각각의 Neutral form 과 Diacid form 의 광물리적 특징을 조사하였다. Absorption spectra 을 통해 Diacid form 이 되면, Neutral 상태일 때보다 Soret band 는 10~20nm Red-shift 하지만, Q-band 는 phenyl group 의 meso 위치가 Methyl 또는 Fluorine 이 치환된 MMMM 과 FFFF 의 경우 Blue-shift 하고 그렇지 않은 TPP 는 Red-shift 하고, AAAA 는 Shift 하지 않는 것은 확인하였다. Fluorescence spectra 에서는 AAAA 가 TPP 와 매우 유사한 것을 확인하였다. 또한, optimized molecular structures 을 DFT 의 RB3LYP Hamiltonian and the 6-31G* basis set 으로 계산하여 electron-withdrawing group 을 phenyl 치환기로 갖는 FFFF, MMMM, PPPP 와 Electron-donating group 을 phenyl 치환기로 갖는 AAAA 를 비교함으로써 치환기 따른 electronic properties 도 확인한다. 이러한 작업을 기초로 하여 얻는 Photophysical properties 와 electronic properties 로 Porphine 과 치환기의 상호작용 및 기하학적 구제에 대한 이해도를 높인다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-334**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Estimation of Lennard-Jones Parameters of Spherical and Cylindrical Molecules from First-Principles Thermodynamics

배현후 최희철[1] 송미영[1,*]

건국대학교 물리학과 [1]국가핵융합연구소 플라즈마기술연구센터

The Lennard-Jones parameters, σ and ε, are fundamental constants to determine thermal conductivity, diffusion collision integral, diffusion coefficient, and so forth, which are used in plasma simulations. The intermolecular potential energy surfaces (IPSs) between homogeneous fluorocarbon gases from ab initio calculations with Basis Set Superposition Error (BSSE) corrections have been explored. Also two parameters σ and ε/k determining the characteristics of pair potential with soft-sphere model were obtained by thermodynamical treatments. In this theoretical work, some known spherical and cylindrical molecules were chosen in order to investigate possibilities for versatile applications of this method, for any types of fluorocarbons. Fluoromethanes($CH_{4-x}F_x$, x=0~4) were picked out to represent spherical-type chemicals and perfluoro-C_2 molecules (C_2F_x, x=2,4,6) were selected as cylindrical ones. Our characteristic parameters are compared with the correponding values obtained from other earlier studies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-335**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Luminescence and magnetic properties of Eu1-xGdx(salen)2 complexes

이지숙

영남대학교 화학과

Complexes of K[Eu1-xGdx(salen)2] (x = 0 – 1.0) were synthesized, and their structural and magneto-luminescent properties were investigated. The complex of K[Eu(salen)2] crystalized in the monoclinic P21/n space group. Exciting the Eu(III) complex with near-UV light resulted in sensitized red luminescence by a energy transfer from the ligand salen to the Eu(III) ion. For K[Eu1-xGdx(salen)2] in acetonitrile, the quantum yield of the sensitized luminescence (Qsens) of x = 0 was 49%. With increasing x, Qsens increased and at x = 0.9 Qsens became the maximum (64 %). Above x = 0.8, with increasing x, Qsens decreased. The molar susceptibility of K[Eu1-xGdx(salen)2] were investigated as a function of x using a MPMS SQUID Magnetometer. The evaluated Curie constant (C) satisified the linear relation of C (emu K) = 5.202.5x + 2.6.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-336**

발표분야: 물리화학

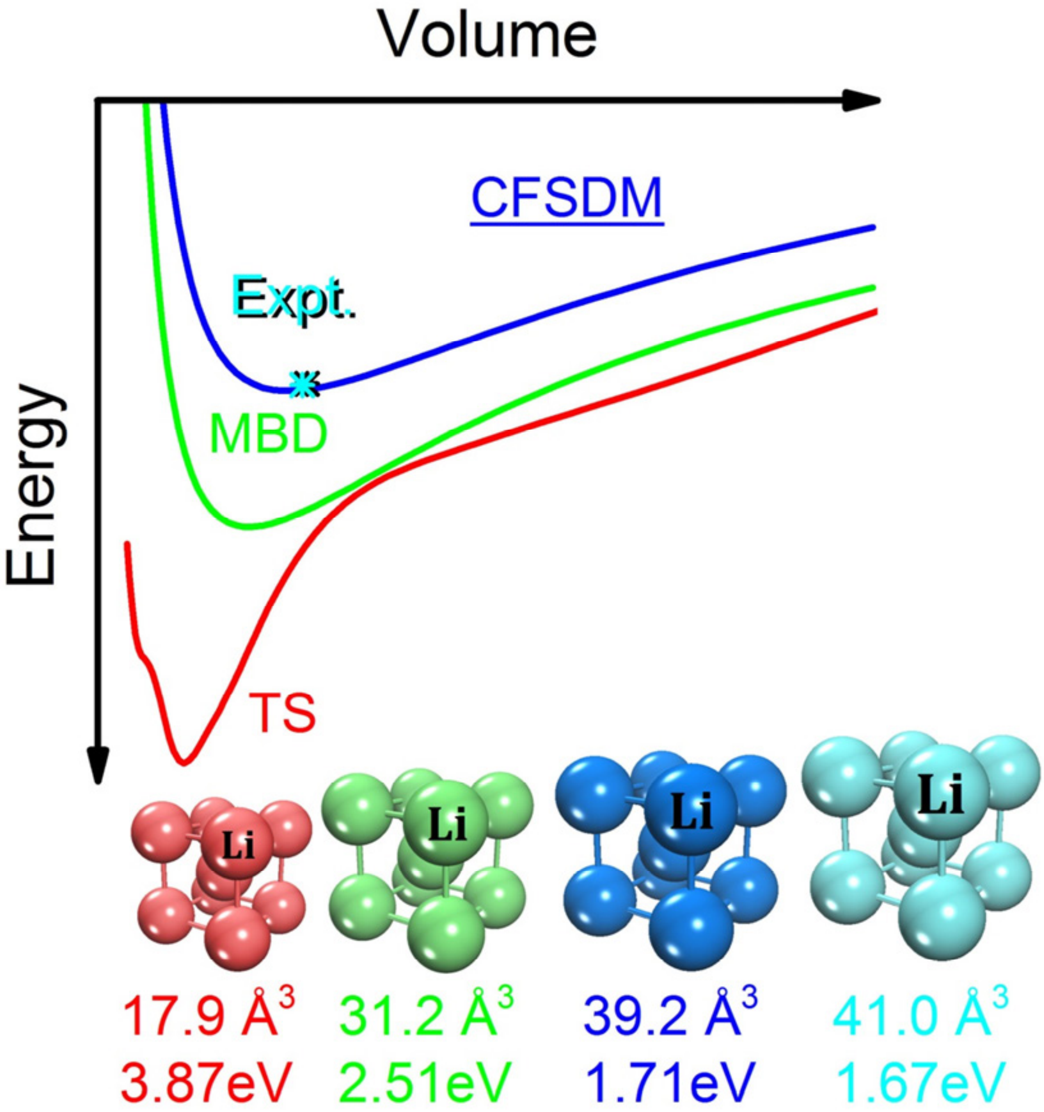
발표종류: 포스터, 발표일시: 목 11:00~12:30

Semiempirical van der Waals Method with a Modified Dipole Model

김민호 김형준*

KAIST EEWS대학원

Previous semiempirical van der Waals corrections to density functional theory lead to an unphysical description of metallic systems, as exemplified by alkali and alkaline earth compounds. We demonstrate that it is possible to remedy this limitation by including screening effects into the form of interacting smeared-out dipoles in the many body expansion of the interaction. Our new approach, called the coupled fluctuating smeared dipole model [1], describes equally well noncovalent systems, such as molecular pairs and crystals, and metallic systems, paving the way for a universal method to describe compounds with diverse type of interactions.[1] W. J. Kim, M. Kim, E. K. Lee, S. Lebègue, H. Kim, *J. Phys. Chem. Lett.* 2016, *7* (16), 3278-3283.


Volume
Energy
CFSDM
Expt.
MBD
TS
Li
Li
Li
Li
17.9 Å3
3.87eV
31.2 Å3
2.51eV
39.2 Å3
1.71eV
41.0 Å3
1.67eV

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-337**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Single-strand DNA binding protein(SSB) displacement from ssDNA by RecO in Deinococcus radiodurans

황지희 이남기[1] 김성근[2,*]

서울대학교 생물물리 및 화학생물학 [1]POSTECH 시스템생명공학부/물리학 [2]서울대학교 화학부

Deinococcus radiodurans (Dr) is the most radio-resistant organism known. It can repair hundreds of double-strand DNA breaks at a time via RecA-mediated DNA recombination. DrRecO is one of major recombination proteins in the RecA-loading pathway, the RecF pathway, and is essential for the extreme radio-resistance of Dr. In this work, we investigated the role of the key component of the RecF pathway using single-molecule spectroscopy. We found for the first time that DrRecO competes with the single-strand DNA binding protein (SSB) in loading ssDNA and can displace SSB from ssDNA, so that it can assist the RecA-loading process.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-338**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Conformationally Resolved Structures of Jet-cooled 2-hydroxyformanilide

문철주 민아름 안아름 성연국 최명룡*

경상대학교 화학과

In this study, we present the conformational investigations and photochemistry of jet-cooled 2-hydroxyformanilide (2-HFA). The number of conformers and their structures of 2-HFA are assigned on the basis of resonance enhanced multiphoton ionization (REMPI), ultraviolet-ultraviolet hole burning (UV–UV HB), infrared-dip (IR-dip) spectroscopy. From comparison between REMPI and UV–UV HB spectra, it was found conformers coexist in the supersonic jet. The structures of these conformers are determined by the IR-dip spectroscopy. Also, the observed spectra are compared with the predictions of ab initio and density functional theory calculations

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-339**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Quantum Chemical Calculations of n-Cyanoindole and its water clusters

안아름 민아름 문철주 성연국 최명룡*

경상대학교 화학과

Franck-Condon integrals are important quantities in physical chemistry. In spectroscopy, they are directly related to the vibronic transition intensities of polyatomic molecules in reaction dynamics, they are used to calculate electron transfer rates in chemical and biological processes. In this study, theoretical calculations of n-Cyanoindole and its water clusters with their size up to 2 water molecules are conducted to aid in the spectroscopic analysis in this laboratory. We calculated the nCI-(H2O)n (n=0-2) clusters using density functional theory (DFT) with a 6-311++G(d,p) basis set and obtained several low minimum energy structures of each nCI-(H2O)n (n=0-2) cluster, including global and low-lying energy local minimum isomers. We further carried out the excited state calculations for the corresponding nCI-(H2O)n (n=0-2) cluster using time dependent-DFT (TD-DFT). Also Franck-Condon simulation for the S0 → S1 transition of nCI-(H2O)n (n=0-2) cluster is presented for the vibrational analysis. The results of Franck-Condon simulations based on DFT ground and excited state geometry optimizations and vibrational frequency calculations showed good agreement with experiment.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-340**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Nickel-Palladium alloy nanoparticles synthesized by pulsed laser irradiation in liquid (PLIL)

정현진 최명룡*

경상대학교 화학과

Among various particle fabrication methods, pulsed laser irradiation in liquid (PLIL) is currently attracting great interest due to its simplicity and versatility. In this study, a two-step process has been employed for the preparation of the Ni-Pd alloy nanoparticles. In the first step, laser pulses at 1064 nm (7 ns at 10 Hz) of a Nd:YAG system were focused to a 99.99% pure nickel plate placed at the bottom of a cell containing methanol. In the second step, laser irradiation using unfocused second harmonic Nd:YAG laser pulses (532 nm, 7 ns, 10 Hz) was applied to the as synthesized Pd-Ni alloy nanoparticles solutions. The Pd-Ni alloy nanoparticles prepared from PLIL were analyzed by X-ray diffraction measurement, field emission-scanning electron microscopy, transmission electron microscopy, and energy dispersive spectroscope.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-341**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Parameters of $LiNiO_2$ for ClassicalMolecular Dynamics SimulationsOptimized by Downhill Simplex Method

이동민 이명원*

부경대학교 화학과

Classical molecular dynamics (MD) is one of the methods that can be used forthe prediction of the properties of systems composed of many atoms. Comparedwith quantum mechanical methods, MD can handle quite large systems veryeffectively, as it requires much less computation time, while quantum mechanicalmethods give more accurate results. In order to obtain more realistic resultsfrom MD simulations, it is crucial to have accurate potential energy functionsused for the systems. In this work, Lennard-Jones potential was used in additionto Coulombic potential to describe $LiNiO_2$ materials, and the parameters inthese potential energy functions were adjusted by downhill simplex method(Nelder-Mead method) so as to closely reproduce quantum mechanical energiesat various structures computed by Quantum ESPRESSO program.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-342**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Time and space resolved LIF detection of OH radical generated by interface electrical discharge

김남주* 강혁[1]

아주대학교 에너지시스템학과 [1]아주대학교 화학과

Because of its high reactivity, OH radical is expected to be useful in air and water purification system but there is a problem that it has short lifetime in the air. Previously, we reported laser induced fluorescence (LIF) detection of OH radical produced by interface electrical discharge with hydrogen gas. In this work we measured temporal and spatial distribution of OH radical produced by the discharge, in order to find out how long the OH radical existed after discharge extinction and how far it can diffuse into surrounding. Electrical discharge was performed by applying AC high voltage across a pair of stainless steel electrodes. A frequency-doubled dye laser (ND 6000, Continum) pumped by the second harmonic of an Nd:YAG laser (Surelite II, Continum) was used to excite v'=1 ← v"=0 transition of OH at 283 nm, and the resulting fluorescence was filtered by a longwave pass filter ($\lambda > 300$ nm) and detected by a photomultiplier tube (PMT). To avoid the background emission from the discharge itself, temporal distribution of OH was measured after the discharge was extinct. Spatial distribution of OH radical was measured by moving the electrodes away from the laser interaction region.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-343**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Free Energy of Lithium Ion un $LiCoO_2$ Computed by Classical Molecular Dynamics Simulations

백성우 이명원*

부경대학교 화학과

$LiCoO_2$ is a common material for the cathode of lithium-ion battery. The cell potential of the battery is related with the free energy of the lithium ion in the electrode materials, and thus predicting the free energy is very important for the development of electrode materials.In the present study, we computed the free energy of the lithium ion from the classical molecular dynamics (MD) simulations of $LiCoO_2$. For the computation of the free energy, we mainly used thermodynamic integration (TI) and free energy perturbation (FEP), which are methods that have been shown to give reliable results. We also computed the free energy using an approximate method, molecular mechanics Poisson-Boltzmann surface area (MM-PBSA), to assess the applicability of this approximate method widely used for the binding free energy calculation of biomolecules. All MD simulations in the present study were carried out with the CHARMM program. The computational results from MD simulations are compared with quantum mechanical and experimental results to check the validity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-344**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electronic Circular Dichroism Spectroscopy of Protonated Ephedrine in a Cold Quadrupole Ion Trap

이슬기 은한준[1] 정창섭[1] 김남준[1,*]

충북대학교 화학과 [1]충북대학교 화학과

We developed a CD spectroscopic technique to obtain the circular dichroism (CD) spectra of jet-cooled chiral molecules, which provided conformation- and vibrational mode-specific CD values. Here, we applied the same CD spectroscopic technique to protonated (*1R,2S*)-(−)-ephedrine ((-)-ED) and (*1S,2R*)-(+)-ephedrine ((+)-ED) produced by electrospray ionization (ESI) to obtain their ECD spectra. The ephedrine ions produced by ESI were stored in a cold quadrupole ion trap and irradiated with circularly polarized laser pulses alternating between left and right (LCP and RCP) generated using a photoelastic modulator. We measured the difference between the fragment ion signals produced by LCP and RCP laser pulses to obtain the electronic CD spectra. We demonstrated that our CD spectroscopic technique can be used to obtain the ECD spectra of molecular ions produced by ESI.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-345**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Induced Circular Dichroism of Jet-cooled Phenol Complexes with Chiral Solvents

홍아람 장희선[1] 문철주[2] 민아름[2] 최명룡[2,*] 허지영[3,*] 김남준[1,*]

충북대학교 화학과 [1]충북대학교 화학과 [2]경상대학교 화학과 [3]상명대학교 의생명공학과

Molecular interactions between achiral and chiral molecules can give rise to circular dichroism within the absorption region of the achiral molecule. This is called induced circular dichroism (ICD) and has been extensively studied in solution. Here, we obtained ICD spectra of jet-cooled phenol complexes with methyl lactate (PhOH-ML) using resonant two-photon ionization spectroscopy (R2PI). The R2PI spectra of PhOH-ML exhibit well-resolved vibronic bands of two different conformers, which is identified using UV-UV hole-burning spectroscopy. The structures of conformers were determined by comparing the IR-UV double resonance spectra with IR frequency predicted by quantum chemical calculations. The origin bands of two conformers show different ICD values and signs. The correlation between the structures of the complexes and ICD effect will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-346**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Induced Circular Dichroism Spectroscopy of Jet-cooled Phenol by Chiral Molecular Interactions

장희선 홍아람 문철주[1] 민아름[1] 최명룡[1,*] 허지영[2,*] 김남준[*]

충북대학교 화학과 [1]경상대학교 화학과 [2]상명대학교 의생명공학과

The binding of a chiral molecule to an achiral molecule induces the circular dichroism (CD) in the absorption region of the achiral molecule, where there is no absorption of the chiral molecule. This is called induced circular dichroism (ICD) and has been extensively studied for many chiral complexes in solution. Here, we obtained the first ICD spectra of phenol-2-butanol complexes (PhOH-BuOH) produced in a supersonic jet using resonant two-photon ionization spectroscopy (R2PI). Two different isomers of PhOH-BuOH present in the jet were identified using UV-UV hole-burning spectroscopy, and the structures were determined by comparing the IR-UV double resonance spectra with the theoretical ones predicted by Time-dependent density functional theory (TDDFT) calculations. The two isomers have different ICD values. We will discuss the relationship between the structures of those complexes and their ICD values.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-347**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparative calculations of the binding strengths of NO and CO molecules on transition metal-ligand complexes

이현주 강준구*

DGIST 신물질과학전공

Nitric oxide (NO) and carbon monoxide (CO) are important neurotransmitters that can alter neuronal activity with potential applications to a variety of neurodegenerative diseases. Therefore, it is crucial to develop NO and CO carriers for delivering the signaling molecules to a target site in a body from outside. Transition metal (TM)-ligand complexes with open TM sites are good candidate systems for molecular carriers. In this theoretical study, we performed hybrid PBE0 calculations to investigate how the adsorption properties of NO and CO depend on the choice of 3d TM elements in TM-ligand complexes (TM = Sc, Ti, V, Cr, Mn, Fe, Co, and Ni). Two model complexes, [TM 3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane]2+ and [TM 1,4,7-trimethyl-1,4,7-triazacyclononane]2+, were considered for our comparative study. We found that for early TMs from Sc to Cr, the binding energy of NO is substantially larger than for the late TMs, ranging from 2.23 eV to 0.22 eV. The largely tunable binding strength arises from different adsorption mechanisms for the early and late TM sites, which are associated with a different magnetic interaction for a TM-NO bond and a charge transfer between TM and NO for early TMs. Unlike the case of NO, the spin degree of freedom does not play a role for the adsorption of a nonmagnetic CO, leading to a relatively narrow range of binding energies from 0.99 to 0.10 eV. Our microscopic understanding of the adsorption mechanisms of NO and CO will provide useful insights into designing efficient neurotransmitter carriers having appropriate binding energies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-348**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Rotation Barrier and Metastable Isomer of Dopdecahedron C20

조용재 이기학[1,*]

원광대학교 바이오나노화학부 [1]원광대학교 화학과, 나노과학기술연구소

We investigate the rotation barrier pattern and metastable isomer of dodecahedron C20 carbon.The staggered form is more stable than the eclipsed form, which is the metastable state.

Rotation Barrier and Metastable Isomer of Dopdecahedron C20

Yongjae Cho and Kee Hag Lee

Motive

- Rotation barrier pattern and the metastable isomer of dodecahedron C20.

Method

- Hybrid Density Functional Theory (B3LYP) method with 6-31g(d) basic set in Gaussian 03W package

Reference

1) Davydov. I.V. ; Podlivaev, A.I ; Openov, L.A phys. Solid State,Vol 47(4),2005,p778-784
2) Katin K P ; Lobanov1 D A ; Maslov M M Journal of Physics: Conference Series 248 (2010)
3) Lin F; Sørensen E.S.; Kallin C; Berlinsky A.J Handbook of Nanophysics : clust5ers and Fullerene 29, 1-11, 2009

Results

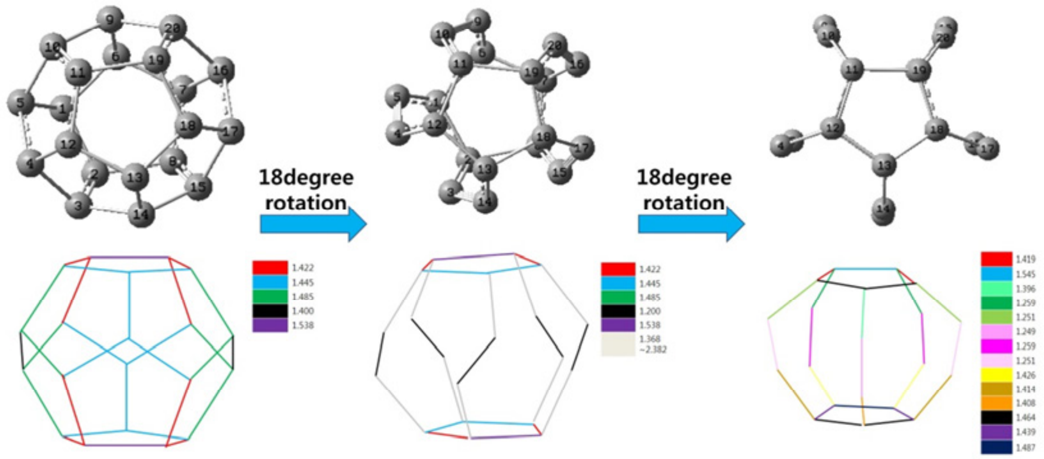


Figure1. Optimized structure of the rotation barrier pattern of dodecahedron C_{20} carbon and bond length

Table 1. The result of B3lyp/6-31G(d)

b3lyp/6-31g(d)	hatree	kcal/mol	eV
0 degree staggered(opt)	-761.4443	-477813.5	-20720.11
18degree half(sp)	-760.8258	-477425.4	-20703.29
36degree half eclipsed(opt)	-761.2877	-477715.2	-20715.86

Table 2. The HOMO and the LUMO energies (eV) and the energy gap (Δe_g) between the HOMO and the LUMO levels (unit: eV)

	HOMO	LUMO	Δe_g
0 degree staggered(opt)	-0.1859	-0.11441	0.07149
18degree half(sp)	-0.21536	-0.16376	0.0516
36degree half eclipsed(opt)	-0.20148	-0.14262	0.05886

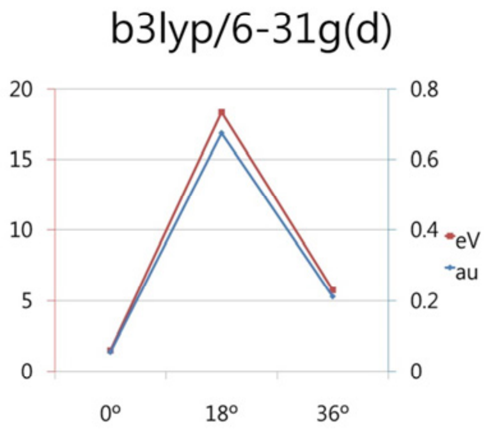


Figure 2. b3lyp/6-31g(d) graph
(ref. ε = -761.5000 for au and 20721.63.00 for eV)

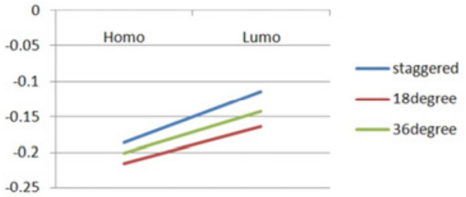


Figure 3. The HOMO-LUMO energy

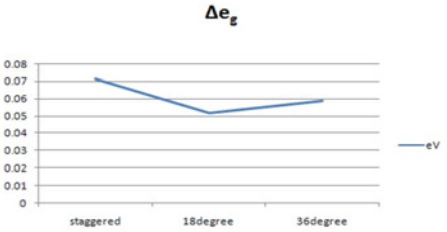


Figure 4. The energy gap (Δe_g) between the HOMO and the LUMO levels (unit: eV)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-349**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Atomic and electronic structure of pyrimidine on group IV semiconductor surface

김도환 홍석륜[1,*]

전북대학교 화학교육과 [1]세종대학교 물리학과

We investigated the chemical reaction of pyrimidine molecule with semiconductor surface using density functional theory (DFT) calculations. The calculations reveal that the dual dative bonding through nitrogen lone pair electrons is the most stable among the possible adsorption configurations. The two N-Ge bonding bridges the two adjacent dimer rows. The energy difference among different geometries depends on the semiconductor atoms and the calculation methods. The experimentally observed STM features were explained on the basis of the electron charge density around the adsorbed pyrimidine molecules and the reacting semiconductor atoms.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-350**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dynamics of laser ablation in liquid phase : the effect of viscosity

김국기 송재규 박승민*

경희대학교 화학과

We examined the laser ablation dynamics of silver target in aqueous phase to explore the effects of liquid phase viscosity on the formation and expansion of laser induced plasma plume bubbles, and nanoparticles. The lifetime of the plasma emission and size of the laser induced bubble decreased with rise the liquid phase viscosity. Also, we check that silver nanoparticles produced by laser ablation in various viscosity range. But, it was impossible to see the TEM image of laser synthesis nanoparticles.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-351**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Photophysical behavior of triazole derivative having tautomeric properties

정연기 김종혁[1] 최창식[2] 이기환[*]

공주대학교 화학과 [1]한국화학연구원 화학분석센터 [2]극동대학교 한약발효학과

The small and simple triazole nucleus containing compounds have received considerable attention owing to their synthetic and effective biological importance. Herein, we report the synthesis, molecular structure, photophysical behavior of 4-(2-fluorophenyl)-3-(3- methoxybenzyl)-1H-1,2,4-triazol-5(4H)-one (5). The structural characterization was performed by using FT-IR, 1H NMR, 13C NMR and single crystal X-ray diffraction analysis. The XRD results showed that the molecule 5 predominantly exists in keto conformation and crystallized in the triclinic system of P-1 space group. The spectroscopic results showed the colorimetric change in the reaction solution and considerable shift in the absorption and emission signal intensity due to the conformational change.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-352**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Homoleptic Cyclometalated Iridium(III) Complexes Based on Phenyl-Imidazole Derivatives : Synthesis, Photodynamic Properties, and Use in OLEDs

김소연 김진형 강상욱[1] 손호진*

고려대학교 신소재화학과 [1]고려대학교 소재화학과

A series of 8 novel homoleptic tris-cyclometalated iridium(III) compounds with phenylimidazole derivatives, $Ir(tpim)_3$ (1a), $Ir(tpdfim)_3$ (2a), $Ir(tpfim)_3$ (3a), $Ir(tpcim)_3$ (4a), $Ir(itpim)_3$ (1b), $Ir(itpdfim)_3$ (2b), $Ir(itpfim)_3$ (3b), $Ir(itpcim)_3$ (4b) : tpim = 1-([1,1':3',1''-terphenyl]-2'-yl)-2-phenyl-1H-Imidazole, tpdfim = 1-([1,1':3',1''-terphenyl]-2'-yl)-2-(2,4-difluorophenyl)-1H-Imidazole, tpfim = 1-([1,1':3',1''-terphenyl]-2'-yl)-2-(4-fluorophenyl)-1H-Imidazole, tpcim = 1-([1,1':3',1''-terphenyl]-2'-yl)-2-(4-cyanophenyl)-1H-Imidazole, itpim = 1-(5'-isopropyl-[1,1':3',1''-terphenyl]-2'-yl)-2-phenyl-1H-Imidazole, itpdfim = 1-(5'-isopropyl-[1,1':3',1''-terphenyl]-2'-yl)-2-(2,4-difluorophenyl)-1H-Imidazole, itpfim = 1-(5'-isopropyl-[1,1':3',1''-terphenyl]-2'-yl)-2-(4-fluorophenyl)-1H-Imidazole, or itpcim = 1-(5'-isopropyl-[1,1':3',1''-terphenyl]-2'-yl)-2-(4-cyanophenyl)-1H-Imidazole, were synthesized and their photophysical, electrochemical properties were reported. The optoelectronic characterization showed a dramatic shift in the emission of the complexes when an electron-withdrawing group was introduced to the ligand. The introduction of electron-withdrawing substituents at 2, 4-position or 4-position of the fluorophenylimidazole ligand emitted blue phosphorescence with • λ_{max} = 455 nm – 480 nm at room temperature (2a, 3a, 2b, 3b). But 4-position of the cyanophenylimidazole ligand showed different behavior in the same condition, a very large bathochromic shift (λ_{max} = 525 nm – 560 nm) was observed in compounds 4a and 4b. DFT calculations accurately modelled the observed photophysical and electrochemical behavior of the complexes and pointed to an emission from a mixed charge transfer state.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-353**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Direct observation of sub-ns frequency correlation decay component in dye dissolved solution system

김준우 주태하*

POSTECH 화학과

Many chemical reactions for research or industry, take place in solution phase. In spite of wide use of solution phase reaction, the detailed dynamics of the reaction is not known to us. Even the development of computational chemistry enabled to understand solution phase reactions, such knowledges are rather energetic rather than dynamic or it requires high cost. The most dominant dynamics in solution phase reaction is the solvation dynamics. Solvation dynamics has been studied by the dielectric response as a result of an electric stimulation. Based on RF and optical response experiments, it has been revealed that the solvation dynamics of small organic solvents complete in 100 ps.Three-pulse photon echo (3PEPS) experiment is an excellent technique which reflects the transition frequency correlation function of a two level system. Thus it is able to measure the solvation dynamics of dye dissolved solution system by virtue of its system-bath coupling. Interestingly, a long-lived frequency correlation has been observed even at the time window after 100 ps. We studied the long-lived component in 2 ns of time window with diffractive-optics based 3PEPS experiment. The decay time of the component is longer than the slowest solvation time and faster than 1 ns. Remarkable feature of the long-lived component is that its decay time is solvent and solute dependent, but is independent to temperature, whereas general solvation dynamics is sensitive to temperature and has negligible solute dependence. This means that the component is neither a pure solvent motion nor a pure intramolecular relaxation. Since the component is correlated to both solvent and solute, it must be a new concept to understand solution phase reaction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-354**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dipolar ejection profile of a new QIT-TOF mass spectrometer

권장한 강혁[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 화학과

Gas-phase laser spectroscopy is one of the good methods to analyze the structures of amino acids and small peptides. However, it is hard to vaporize and freeze the biomolecules with the conventional heating method, because they are prone to thermal fragmentation. In order to overcome the restriction in the size of the molecules that can be vaporized, we are constructing a new ESI (electrospray ionization) - QIT (quadrupole ion trap) - TOF (time-of-flight) mass spectrometer (MS). When there are several types of ion with different m/z in the QIT, sometimes it is necessary to eject one type of ion from QIT. For example, in a double-resonance spectroscopy of an ion, the parent ion and its daughter ion by a burn laser are both present in QIT, and it is necessary to eject the fragment ion from the QIT before irradiating a probe laser. Dipolar auxiliary RF (tickle RF) can be used to excite the secular motion of a specific ion that is resonant with the frequency of tickle RF and finally to eject it from QIT. We have modified the QIT to apply tickle RF to the entrance end cap of the QIT and optimized the ejection efficiency by adjusting the frequency and voltage of tickle RF and trapping time of QIT.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-355**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Low temperature study of sodium chloride in ice using terahertz time-domain spectroscopy and fourier transform infrared spectroscopy

박재헌

POSTECH 포항가속기연구소/빔라인부

The molecular interaction of ionic materials in a liquid- or ice- structure of water has been investigated for over five decades. To find the properties related to the inter- and intra-molecular interaction, terahertz time-domain spectroscopy and fourier transform infrared spectroscopy have been studied. In the THz frequency range, there is a broad stretch mode of ice at 5 THz and no resonance of other modes below 5 THz due to strong hydrogen bonds in crystalline water. The absorption peak of stretch vibration of -OH and -OD group in ice is detected at 3500 cm-1 and 2500 cm-1, respectively. These resonance peaks are changed by an ionic polar material added to crystalline water because the structure of ice is disordered by impurities. In this study, we shows the change of the absorption peaks of sodium chloride in ice as a function of temperature at THz and IR frequency ranges and discuss the relationship between the inter- and intra-molecular vibrations.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-356**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optimum Diameter of Silver Colloid Particles for Surface Raman Scattering

윤혁진 서정쌍*

서울대학교 화학부

We have studied the optimum size of spherical silver colloid particles for surface-enhanced Raman scattering (SERS). Four different diameters of spherical silver nanoparticles were fabricated by a seed-mediated process. Their average diameters were 20, 25, 29, and 32 nm. We fabricated SERS substrates consisting of the clusters of silver colloid particles using a three-step immobilization method: immobilized colloid particles on cover glass coated with poly(4-vinyl pyridine), and adsorbed target molecules on the immobilized particles, and then immobilized colloid particles again. A good SERS spectrum was observed from the substrates by excitation with the 514.5 nm laser line, and the SERS intensity was affected by the diameters of Ag colloid particles. Ag colloid particles whose average size was 29 nm showed the highest intensity. The calculated highest enhancement factor was about 1x107 which was about 10 times better than that whose Ag colloid particle size was not optimized.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-357**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optimal dimension of discrete variable representation for mixed quantum/classical computations of OH vibration and its anharmonicity in liquid water

전기영 양민오*

충북대학교 화학과

Three low-lying vibrational states of molecular systems are responsible for the signals of linear and third-order nonlinear vibrational spectroscopies. Theoretical studies based on mixedquantum/classical calculations provide a powerful way to analyze those experiments by simulating their signals. To obtain a meaningful result from the calculations, the three vibrational states should beobtained by solving the Schrödinger equation over a numerous number of molecular configurations. The discrete variable representation (DVR) method is a powerful computational technique to calculatevibrational eigenstates subject to an arbitrary anharmonic potential surface. Considering the large number of molecular configurations over which the DVR calculations have to be repeated, the calculationsare desired to be optimized between the cost and accuracy. In this presentation, we determined an optimal dimension of the DVR method to calculate the three states of molecular vibrations with anharmonicstrengths often found in realistic molecular systems. We applied the numerical technique to calculate the OH stretching frequencies of liquid water which are well known to be widely distributed due toinhomogeneity and found that the inhomogeneous frequencies of the 0-1 and 1-2 transitions are highly correlated. An empirical formula for the anharmonicity frequency is suggested in terms of thefundamental transition frequency.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-358**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Studying Water Hydrogen-bonding Network near the Lipid Multibilayer with Multiple IR probes

<u>KUNDU ACHINTYA</u> 조민행*

고려대학교 화학과

Water near the membrane surface is a biological environment for many biochemical reactions and maintenance of the structural integrity of the membrane. Therefore, molecular level understanding of water structure and dynamics near the membrane is prerequisite to perceive the role of water in such relevant biological environment. The OD stretch mode of HOD molecules as IR probe was used to study the water dynamics at the lipid multibilayer (mimic the biological membrane) using femtosecond IR pump-probe spectroscopy [1,2]. The azido stretch mode of HN3 is a promising IR probe for studying local water structure in confined systems due to its narrow spectral bandwidth and large transition dipole moment [3]. Here, we used two different IR probes (OD stretch mode and azido stretch mode) to study water hydrogen-bonding structure and dynamics near the lipid multibilayer. We observed two distinct vibrational lifetime components of OD stretch mode of HOD molecule near the lipid multibilayer. The fast component (0.6 ps) is associated with water interacting with the phosphate moiety, whereas the slow component (1.9 ps) is bulk-like choline-associated water. However, with azido probe, we observed only bulk-like choline-associated water. Because of the tight packing of the head part of the lipid in the gel phase, HN3 molecules mostly stay at the very end part of the lipid (in the bulk region). Indeed, the vibrational lifetime (～2.4 ps) is close to azido stretch of bulk HN3 (～2.5 ps). We anticipate these different type of water near the lipid multibilayer have an important role for many biochemical reactions at these biological environment. References:[1] Kundu, A.; Bartosz, B.; Lim, J.; Kwak, K.; Cho, M. J. Phys. Chem. Lett. 2016. 7, 741. [2] Zhao, W.; Moilanen, D. E.; Fenn, E. E.; Fayer, M. D. J. Am. Chem. Soc. 2008, 130, 13927.[3] Lee, J.; Maj, M.; Kwak, K.; Cho, M. J. Phys. Chem. Lett. 2014. 5, 3404.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-359**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of the Ancillary Ligands on the Heteroleptic Iridium(III) Complexes: A Combined Experimental and Theoretical Study

조양진 김소연 강상욱[1] 손호진[*]

고려대학교 신소재화학과 [1]고려대학교 소재화학과

The non-radiative decay of the high energy triplet state of a series of Ir(III)-complexes associated with the cleavage of one M–L bond was examined by integrating quantum chemical modeling methods and various experimental techniques. Quantum chemical models suggest that the deep blue phosphorescence originates mainly from a ^{3}MLCT excited state. A chemical pathway for the non-radiative decay from the ^{3}MLCT state involving a M–L bond cleavage is explicitly modeled and complete reaction cycles were constructed. Heteroleptic complexes were prepared by employing acetylacetonate (acac), picolinate (pic) and tetrakis-pyrazolyl borate (bor) as ancillary ligands to investigate the stability of the emissive triplet state. Among these heteroleptic complexes, $\mathrm{Ir(dfCF_3)_2(bor)}$ ($\mathrm{dfCF_3}$ = 2-(2,4-difluoro-3-(trifluoromethyl)phenyl)-4-methyl-pyridine) showed emission lifetime of 4.36~4.77 μs, it is less dependent on temperature (20~70 $^{\circ}$C). Otherwise $\mathrm{Ir(dfCF_3)_2(acac)}$ showed emission lifetime of 0.420~1.15 μs, which is more dependent on temperature. A detailed analysis of the computational model and time-resolved luminescence experiments suggest that a combination of electronic effects and the bulkiness of the borate ancillary ligand protect the radiative excited state from non-radiative decay. Finally, $\mathrm{Ir(dfCF_3)_2(bor)}$ was tested as dopants in prototype phosphorescent organic light-emitting diode devices and found to show deep blue electroluminescence with high emission efficiency and color purity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-360**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Vibrational relaxation of the HCO_2CH_3 in CCl_4

김성훈 임만호[1,*]

POSTECH 포항가속기연구소 [1]부산대학교 화학과

The vibrational relaxation of the C=O stretching mode of the HCO_2CH_3 in CCl_4 solution at room temperature were measured using femtosecond infrared spectroscopy. Time-resolved spectra after excitation of the C=O stretching mode reveal a new absorption other than that from the v=1 state of the C=O mode. The amplitude of the new absorption initially grows and then decays with the pump-probe delay time. The recovery of the bleach is somewhat slower than the decay of the transient excited-state absorption. The kinetics of the bleach and excited-state absorption show nonexponential decay with fast and slow component. At longer than 1 ps time delay, the vibrational relaxation dynamics can be well described with three-state model. Apart from the slow decay component, the fast subpicosecond decay is observed and may be caused by the solvent memory effects.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-361**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The influence of p-conjugation on competitive pathways: charge transfer or electron transfer in new D–π–A and D–π–Si–π–A dyads

조양진 김소연 한원식[1] 손호진 조대원 강상욱[2,*]

고려대학교 신소재화학과 [1]서울여자대학교 화학과 [2]고려대학교 소재화학과

In order to elucidate the influence of π-conjugation on photoinduced electron transfer (PET) and intramolecular charge transfer processes, donor–π–acceptor dyads (D–π–A (1) and D–π–Si–π–A (2)) were newly synthesized. In these dyads, carbazole and triazine moieties acted as the electron donor and acceptor, respectively. The fluorescence of dyad 1 red-shifted as the solvent polarity was increased. The electron charge distribution of the excited state of dyad 1 was delocalized in the acceptor moiety, forming the charge transfer $D^{\delta+}$–π–$A^{\delta-}$ dyad in the excited state. In the excited state of dyad 1, the π-conjugation acted as the linker for charge transfer between the donor and acceptor moieties. A large dipole moment change ($\Delta\mu = 45.6$ D) between the ground and excited states was determined using the Lippert–Mataga plot. Furthermore, the fluorescence of dyad 1 was observed upon two-photon excitation. In contrast, dyad 2, in which the π-conjugation is disconnected by a Si-atom in the linker, displayed weak dual-emission: a short-wavelength emission at around 350 nm arising from the monomeric species and a long-wavelength one assigned to the emission from an intramolecular exciplex between the donor and acceptor moieties. The weak emission of dyad 2 indicates that the $D^{+\cdot}$–π–Si–π–$A^{-\cdot}$ species was generated through a PET process in the excited state. The cationic radical species of the carbazole and the anionic radical species of the triazine, which show transient absorption (TA) bands at around 780 and 530 nm, respectively, were characterized using the femtosecond TA method.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-362**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ligand-to-ligand charge transfer in heteroleptic Ir-complexes: comprehensive investigations of its fast dynamics and mechanism

조양진 김소연 위경량[1] 손호진 한원식[2] 조대원 강상욱[3,*]

고려대학교 신소재화학과 [1]대구대학교 화학응용화학과 [2]서울여자대학교 화학과 [3]고려대학교 소재화학과

To gain new insights into ligand-to-ligand charge-transfer (LLCT) dynamics, we synthesised two heteroleptic Ir^{3+} complexes: ($Ir(dfppy)_2(tpphz)$) and ($Ir(dfppy)_2(dpq)$), where dfppy, tpphz, and dpq are 2-(4,6-difluorophenyl)pyridine, tetrapyrido[3,2-a:2',3'-c:3'',2''-h:2''',3'''-j]phenazine, and 2,3-bis-(2- pyridyl)-quinoxaline, respectively. The tpphz and dpq ligands have longer π-conjugation than dfppy. Therefore, the excited ligand-centred (LC) state and the metal-to-ligand charge transfer (MLCT) state of dfppy are higher than those of tpphz and dpq. The LLCT dynamics from dfppy to tpphz (or dpq) was probed using femtoscond transient absorption (TA) spectroscopy after the selective excitation of dfppy. The TA band for the LC/MLCT state of dfppy is observed at 480 nm. Because of the LLCT process, the TA bands related to the MLCT states of tpphz and dpq ligands increased, whereas those of dfppy decreased. The time constants for the LLCT process were 17 ps for $Ir(dfppy)_2(tpphz)$ and 5 ps for $Ir(dfppy)_2(dpq)$. The MLCT emission of $Ir(dfppy)_2(tpphz)$ showed strong temperature dependence, indicating that the LLCT process has a significant energy barrier. In comparison, the temperature weakly influenced the emission of $Ir(dfppy)_2(dpq)$, and thus, its LLCT process may have a smaller barrier. The anomalous rigidochromism and photodynamic behaviours can be explained in terms of the barrier between cyclometalating and ancillary ligands.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-363**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Aggregation-induced emission of diarylamino-π-carborane triads: effects of charge transfer and π-conjugation

조양진 김소연 한원식[1] 손호진 조대원 강상욱[2,*]

고려대학교 신소재화학과 [1]서울여자대학교 화학과 [2]고려대학교 소재화학과

Carborane-based donor–π–acceptor triads (D–π–A–π–D) bearing triarylamine moieties were synthesised. All the monomeric triads showed a blue-green emission in a dilute solution, which was assigned as an intramolecular charge-transfer (CT) emission. The intramolecular CT emission showed large Stokes shifts at a higher solvent polarity. The intramolecular CT emission further shifted to a longer wavelength with the increase in π-conjugation. Interestingly, a strong red emission was observed in highly concentrated solutions or in the solid state, which was assigned as an aggregation-induced emission (AIE). Moreover, the AIE strongly depended on solvent polarity. A large Stokes shift in AIE was attributed to the strong CT character. The changes in the dipole moment for the AIE state and monomer emission were evaluated using the Lippert–Mataga relationship. The density functional theory calculations showed that the change in electron distribution between the aryl amino group (highest occupied molecular orbital, HOMO) and the carborane moiety (lowest unoccupied molecular orbital, LUMO) indicates the intramolecular CT character, and the emission colour changes were attributed to the HOMO–LUMO energy gap controlled by the π-extension of the phenylene linker. The electrochemical properties such as oxidation and reduction potentials were consistent with theoretical calculation results. The emission properties were affected by two main factors: solvent polarity and solubility.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-364**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Single-gold-atom catalyst adsorbed on graphite and potassium-intercalated graphite for CO oxidation

이민희 정재훈*

울산대학교 화학과

Single-atom catalyst is recently receiving much attraction as a novel heterogeneous catalyst. Here, we investigate the catalytic activity of atomic gold for the CO oxidation using periodic density functional theory (DFT) calculations. Two types of support materials, graphite (Gr) and K-intercalated graphite (K@Gr), with a single vacancy (SV) were employed as a model system. SV not only plays a role in introducing the isolated gold atoms on the support materials but also influences the charge redistribution near individual gold atoms. We examined two CO oxidation processes, Eley-Rideal and Langmuir-Hinshelwood mechanisms, on both support materials, respectively. We expect that our computational results provide deeper insight into controlling catalytic reactivity for designing new catalytic system.

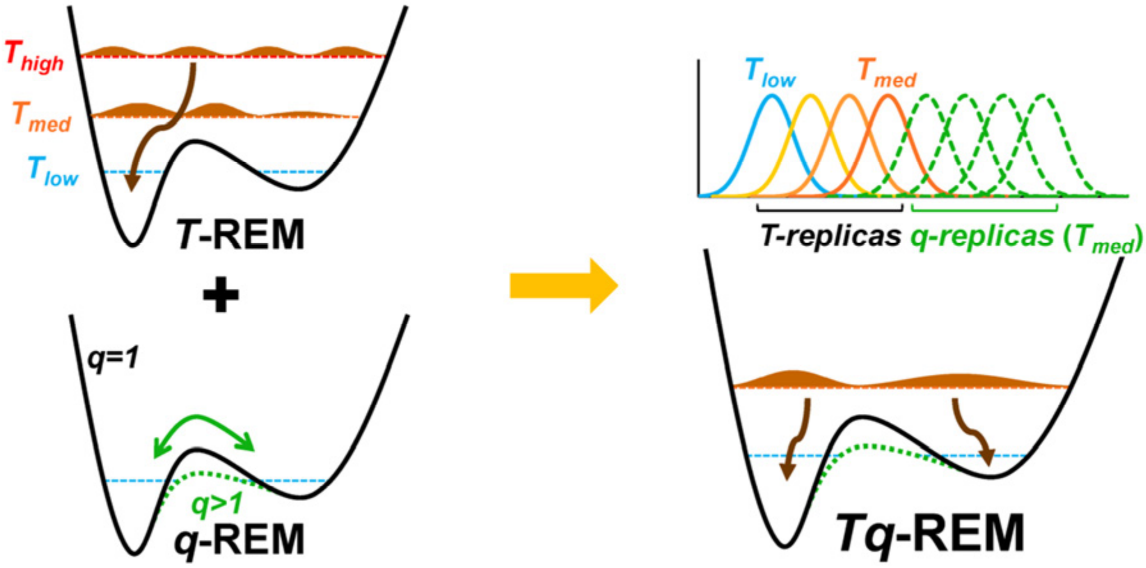
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-365**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tq-REM: Novel Replica Exchange Method for Conformational Sampling of Metastable States

이민준 윤제성 장순민[1] 신석민*

서울대학교 화학부 [1]세종대학교 화학과

Replica exchange methods (REMs) have been extensively used as efficient conformational sampling methods for bio-molecular simulations. However, their application to very large bio-systems are somewhat limited. We propose a new replica exchange scheme (*Tq*-REM) created by combining the conventional temperature-REM (*T*-REM) and one of the Hamiltonian-REMs, *q*-REM, using the effective potential with reduced barriers. In the proposed *Tq*-REM scheme, high temperature replicas in *T*-REM are substituted with *q*-replicas. This combined scheme is expected to exploit advantages of the *T*-REM and *q*-REM resulting in improved sampling efficiency while minimizing the drawbacks of both approaches. We investigated the performance of *Tq*-REM compared with *T*-REM by performing all atom MD simulations on Met-enkephalin, $(AAQAA)_3$, and Trpzip2. It was found that convergence of the free energy surfaces was improved by *Tq*-REM over the conventional *T*-REM. In particular, the trajectories of *Tq*-REM were able to sample the relevant conformations for all of the metastable folding intermediates, while some of the local minimum structures are poorly represented by *T*-REM. The results of the present study suggest that *Tq*-REM can provide useful tools to investigate systems where metastable states play important roles.


T_{high}
T_{med}
T_{low}
T-REM
+
q=1
q>1
q-REM
T_{low}
T_{med}
T-replicas
q-replicas (T_{med})
Tq-REM

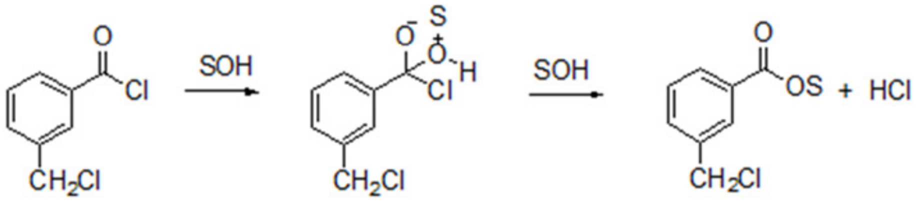
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-366**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Analysis of the solvolytic reaction mechanism of 3-(Chloromethyl)benzoyl chloride

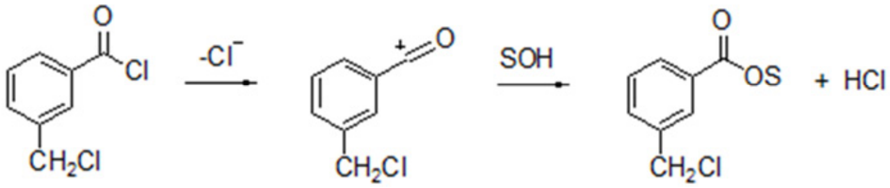
김세린 박경호[1,*]

한양대학교 응용화학과 [1]한양대학교 과학기술대학 응용화학과

The measuremet of the rate constants of 3-(chloromethyl)benzoyl chloride(1) has gained at 25.0℃. The solvents was consisted with the pure ethanol, methanol, 2,2,2,-trifluoroethanol(TFE) and the binary aqueous mixture of ethanol, methanol, TFE. Also the binary solvents with the acetone, 1,1,1,3,3,3-hexafluoro-2-propanol(HFIP) and water, and the mixture of ethanol and TFE was used. The analysis of the rate constants, performed by the extended Grunwald-Winstein equation. Also, the activation parameters can support to understand how the reaction go through. The plot of data including all solvents has large dispersion. It is the reason we divide the solvents in two systems. The l and m values in the nucleophilic solvent are 1.24 and 0.43 respectively, while the l and m values in the electrophilic solvents -except the TFE-EtOH mixture- are 0.47 and 0.76 respectively. Additionally, we gain the activation parameters, the enthalpy is 14.4~18.3 and entropy is -14.3~-0.4. With these process, we decide that the solvolysis of 1 has two different pathway in two solvent systems. In the nucleophilic solvents 1 has a bimolecular pathway. On the other hand, 1 has a unimolecular mechanism when the reaction occurs in the electrophilic solvents. Also, we compared the result with the data of 4-(chloromethyl)benzoyl chloride(2), we studied previously, and deduce the reaction mechanism. When we compared the 1 with 2, there were little difference at the outcomes. This shows that the chlorine which attached at the methyl substituent does not affect the reaction mechanism. Unfortunately, there are few studies about the meta-substituent benzoyl chloride. It should be studied more about the mechanism of the meta- substituent benzoyl chloride.



Schem1. Bimolecular pathway in nucleophilic solvents



Schem2. Unimolecular pathway in electrophilic solvents

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-367**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Chiral Differentiation of *D*- and *L*-Alanine by Permethylated β-Cyclodextrin: IRMPD Spectroscopy and DFT Methods

이성식 오한빈[1,*] 이성렬[2,*]

경희대학교 국제캠퍼스 화학과 [1]서강대학교 화학과 [2]경희대학교 응용화학과

Gaseous chiral differentiation of alanine by permethylated β-cyclodextrin is studied using IRMPD spectroscopy and density functional theory calculations. The protonated non-covalent complexes of permethylated β-cyclodextrin and the D- or L-alanine were mass-selected and investigated by IR laser pulses in the wavelength region of 2650-3800 cm^{-1}. The remarkably different features of the IRMPD spectra for D- and L-alanine are described, and their origin is elucidated by quantum chemical calculations. We show that the differentiation of the experimentally observed spectral features is the result of different local interactions of D- and L-alanine with permethylated β-cyclodextrin. We also assign the extremely high-frequency (>3700 cm^{-1}) bands in the observed spectra to the stretch motions of the completely isolated alanine –OH groups.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-368**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Contribution of noncovalent intermolecular interactions to the formation of supramolecular complexes

오지훈 지기환* 정재훈*

울산대학교 화학과

The supramolecular architectures, such as catenanes, trefoil, and pentafoil knots, Solomon links, and Borromean rings, has received a great scientific interest as a potential material for host-guest chemistry, selective sensing, drug delivery, and anticancer studies. Recently, the successful syntheses of Solomon links [1] and Borromean rings [2] with unique architectures were reported by Chi et al., which are composed of the tetracene-Ru(II) acceptor and carbazole-functionalized donor, and ditopic pyridyl donor, respectively. We carried out the computational study based on density functional theory in order to provide the rationale for the formation of supramolecular complexes. For the sake of reliable comparison, we evaluated the binding energies with three different hybrid density functionals, PBE0, M06-2X, and ωB97X-D, in which, whereas PBE0 cannot describe van der Waals interactions, both M06-2X and ωB97X-D were designed to effectively deal with the weakly interacting systems. The formation of supramolecular complexes, both Solomon links and Borromean rings, can be reasonably explained by the geometrical configuration with effective noncovalent intermolecular interactions, i.e., C-H…π and π…π interactions. Our computational results provide a fundamental insight into the formation of supramolecular complexes, the newly synthesized Solomon links and Borromean rings.

1.Y. H. Song, N. Singh, J. Jung, H. Kim, E.-H. Kim, H.-K. Cheong, Y. Kim, and K.-W. Chi, Angew. Chem. Int. Ed. 55, 2007 (2016).
2.T. Kim, N. Singh, J. Oh, E.-H. Kim, J. Jung, H. Kim, and K.-W. Chi, J. Am. Chem. Soc. 138, 8368 (2016).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-369**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Computational Simulation Spectral Analyses of Lanthanide and Actinide Complexes

정태섭 이경구[1,*] 차완식[2,*] 배상은[3,*] 곽경원[*]

고려대학교 화학과 [1]군산대학교 화학과 [2]한국원자력연구원 원자력화학연구부 [3]한국원자력연구소 화학연구부

Spectral analyses of the lanthanide and actinide complexes are essential part for the remote detection of leaking of radioactive stream. However, there is riskiness that caused radioactivity during experimental approaches to obtain radioisotope spectra especially in actinide complexes cases, therefore the virtual screening using advanced simulation techniques has been proposed and extensively used to reduce the chance of exposure to radioactive materials. Here, we perform the computational investigations for the complexes, especially samarium chloride complexes. All of simulations are accomplished using Gaussian 09 program package with mPW1LYP, and mPW1PW91 functional and the levels of basis set are 6-311++G(3df,3pd) for ligand and the Wood-Boring quasi-relativistic method(MWB) for center metal atom. We optimized some complex structures, and simulated their UV-Vis spectra. Through the natural transition orbital(NTO) research, we could assign their peaks on the spectra to their electronic transition.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-370**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Reactive oxygen species and *Monascus purpureus* pigments*

송유진 김용록*

연세대학교 화학과

Red yeast rice, which is a staple food in Asia, is made by fermenting the fungi on rice. *Monascus purpureus* (MP) in genus *Monascus*, one of the fungi, is the most widely used for rice fermentation due to its antioxidant properties of the natural pigments (red, orange, yellow) as secondary metabolites. In this work, the photophysical properties of the *Monascus purpureus* pigments (orange, red) were confirmed by using steady-state absorption and emission spectroscopy. And the antioxidant efficiency and singlet oxygen, which is one of the reactive oxygen species (ROS), generation efficiency of the natural pigments were estimated with the time and wavelength-resolved singlet oxygen phosphorescence spectroscopy. The singlet oxygen quenching rate constants of each pigment were calculated with Stern-Volmer plotting. It is hoped that the quantized singlet oxygen generation and quenching efficiency of natural pigments provide the useful information in food industry. *This work has been collaborated with the groups of Prof. Chul Soo Shin and Prof. Kyoung Tai No, Dept. of Biotechnology, Yonsei University, Seoul, Republic of Korea.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-371**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Measurement of Raman scattering signals for toxic chemicals using deep UV laser

<u>고영진</u>* 이재환[1] 정영수[1] 이준오[1]

국방과학연구소 5-3 [1]국방과학연구소 5본부 3부

The Raman spectroscopy is an attractive method for the identification of chemicals with similar structure and widely used for the analysis of materials. The technique allows remote detection, non-destructive and fast sensing. Due to advanced ultraviolet light source technology, the Raman spectrometer based on ultraviolet laser has been actively developed, recently. In case of using below 250 nm wavelength as a deep UV light source, it is easy to measure the Raman spectra by spectrally seperating the Raman and the fluorescence.In this research, we measure of Raman scattering signals for toxic chemicals on various deep UV wavelength and compared with Raman spectra according to laser wavelengths.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-372**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Interlayer Interactions and Stacking Structures of Graphene-based 2D Materials

전병선 이상욱[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 응용화학과

Since graphene has developed, two-dimensional material systems have attracted tremendous interest from many researchers in the various nanotechnology research fields. Because of its outstanding properties, scientists have tried to synthesis new two-dimensional materials based on graphene. Recently, two dimensional crystal with uniform sp^2 hybridization holey nitorgenated graphene structure, called as C_2N-*h*2D, has been developed by bottom-up wet-chemical reaction. This newly synthesized two-dimensional crystal is expected to be used for various applications as energy electrodes, semiconductor device, catalyst and gas storage. To applicate this new material, we must know the exact structure of it, so we have tried to find its three dimensional stacking configuration. In this work, we found that there are seven different stacking types of C_2N-*h*2D and ABC stacking order is the most stable structure of it.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-373**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Juxatamembrane domain of c-KIT mutant: Structure, Function and Role in the receptor tyrosine kinase

김철희 김은애*

조선대학교 약학과

c-KIT is a type III family of the receptor tyrosine kinases and is associated with Acute Myeloid Leukemia (AML), GastroIntestinal Stromal Tumor (GIST), and germ cell tumors. The mechanism of action starts to receive a signal of Stem Cell Factor (SCF) on extracellular and then proceeds with the dimerization of c-KIT. The receptor of dimer activates the signal transduction through JAK, PI3K, RAS and SFK pathway simultaneously. However, the mechanism of c-KIT mutant is different with that of the wild-type c-KIT. The single mutation in Active-loop (A-loop; residues 810-835) of the c-KIT affects a downstream pathway and drug resistance to Imatinib (Gleevec).

In this study, we carried out the molecular dynamics (MD) simulation and analyzed the structural change of the mutants (D816V and N822K in A-loop) compared with the wild-type c-KIT. We considered about two system; the mutant with juxatamembrane region (JMR; residues 547-558), the mutant without JMR. All NVT simulations run at 310K and the data were fully converged. To investigate the interaction of intra-motif, we calculated the sidechain contacts and the cluster analysis. As a result, the structure of the wild-type c-KIT doesn't matter what is with JMR or without JMR. However, the structure of the mutant without JMR is different with that of the mutant with JMR. Therefore, the JMR of the mutant would play an important role due to the rearranged interaction of intra-motif.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-374**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Doping Effect on Graphene Nanoribbons, Terminated with Organic Radicals

남연식 조대흠 이진용*

성균관대학교 화학과

Doping effect on intramolecular magnetic exchange coupling of zigzag graphene nanoribbon (ZGNR) terminated with organic radicals, was studied with density functional theory. We introduced boron (B) and nitrogen (N) on ZGNR, terminated with trimethylenemethane (TMM) and 6-oxoverdazyl (OVER) radicals, i.e., TMM-ZGNR-TMM, OVER-ZGNR-OVER, and TMM-ZGNR-OVER along with the shortest magnetic coupling pathway and investigated their magnetic property changes: magnetic ground configuration, magnetic coupling strength, and magnetic moment.The first doping switched the magnetic ground configuration of a system from antiferromagnetic (AFM) to ferromagnetic (FM) and vice versa. An additional doping switched it back to its original magnetic configuration. For magnetic coupling strength, N doping on edge increased the magnetic coupling strength as compared with the undoped system, while B doping decreased it. Furthermore, doping on TMM-terminated edge increased the magnetic moment of the system, while the same doping on an OVER-terminated edge decreased it either B or N. Our results demonstrate a possibility of reversible spin control of organic magnetic materials by chemical doping.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-375**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of Size and Structure on the Ground and Excited StateElectronic Structure of Small TiO2 Clusters and Nanoparticles

조대흠 이진용*

성균관대학교 화학과

We investigated the influence of size and structure on the electronic structure of 0.5-3.2 nm diameter TiO2 nanoparticles in both vacuum and water using density functional theory calculations. Specifically, we tracked the optical and electronic energy gap of a set of (TiO2)n nanoparticles ranging from small non-bulk-like clusters with n =4, 8 and 16, to larger nanoparticles derived from the anatase bulk crystal with n = 35 and 84. As the difference between these two energy gaps (the exciton binding energy) becomes negligible in the bulk, this magnitude provides an indicator of the bulk-like character of the electronic structure of the nanoparticles under study. Our results generally confirmed that the electronic structure of nanoparticle ground state and excited state has a more pronounced structure dependency than size dependency within 0.5-1.5 nm size. We also showed that thermodynamic preference for the photocatalytic species is the first S1 exciton. This S1 exciton is stable in vacuum but may evolve to free charge carriers upon structural relaxation in an aqueous environment for 0.5-1.5 nm size particles studied in the present article. An analysis of ionization potentials and electron affinities relative to the standard reduction potential for the water splitting half-reactions revealed the importance of considering the structural relaxation in the excited states and the presence of water for assessing the thermodynamic conditions for photocatalytic water splitting.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-376**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Kinetics and Mechanism of Schiff Base Hydrolysis for Water Sensor in Organic Solvents

SHIHU 조대흠 김종승[1,*] 이진용[*]

성균관대학교 화학과 [1]고려대학교 화학과

Traditional methods have several drawbacks, such as the cost of operation and instrumentation and their time-consuming nature, for the quantification of water content in gas streams or liquid phases. Recently, optical sensors for detecting water contents have received substantial attention due to the possibility of remote and in situ monitoring as well as their cost-effective fabrication. In the current study for molecular design, coumarin was used as the fluorophore skeleton and derivatives of aniline and pyridine were introduced as Schiff bases, as they not only extend the conjugation inducing a fluorescence shift but also enhance the fluorescence intensity. Our results show that reactivity of probe 6 clearly outperformed the other probes (3, 4, and 5) in DMSO solution. Furthermore, the absorption band of 6 showed only a slight solvent dependency, indicating 6 could potentially be used as a water sensor in a range of organic solvents. The kinetics study in buffer solutions at various pH levels revealed that the hydrolysis of 4 and 6 was remarkably enhanced in acidic solutions, in contrast to basic solutions. DFT and TDDFT were used to gain a better mechanistic insight into the pH dependent reaction rate. In acidic solutions, the second dissociation step is barrierless, while in basic solutions, the first water addition step is barrierless. In neutral solutions, for both 4 and 6, the water addition is the rate determining step. It can clearly be seen that the activation barriers for the hydrolysis of 6 are lower than for 4, which is consistent with the kinetic data obtained from the time-dependent fluorescence changes. It can be concluded that the hydrolysis can be much enhanced in acidic solutions as noted from the greatly reduced activation barrier as compared to neutral solutions. The calculated energy profile is in excellent agreement with experimentally observed pH dependent kinetics. Thus, probe 6 would most effectively work as a water sensor in acidic solutions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-377**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A DFT study on single oxygen vacancy in $(TiO_2)_{35}$ anatase nanoparticle: Implication to photocatalytic activity

김선경 **FRANCIS KIRBY BURNEA** 이진용*

성균관대학교 화학과

Titanium dioxide (TiO_2), as a semiconductor metal oxide, has been one of the most popular materials studied in the field of photocatalysis. In the present study, the properties of single oxygen vacancies of $(TiO_2)_{35}$, a prototype of anatase nanoparticle, were investigated by DFT calculations. $(TiO_2)_{35}$ is the minimum sized model (~ 2 nm) as bipyramidal nanoparticle with anatase phase and eight {101} facets. All the available oxygen vacancies at various sites according to position, coordination number, and distance from the center atom were examined. The geometric, energetic and electronic properties of the reduced TiO_2 clusters were analyzed by hybrid DFT functionals with different Hartree-Fock exchange ratio (0, 12.5 and 25 %). It was found that the structure of pristine $(TiO_2)_{35}$ is somewhat different from bulk lattice with relatively high surface to volume ratio. Moreover, the particular high (three)-coordinated oxygen atom is energetically most favorable for oxygen vacancy formation from nanoparticle mainly due to substantially high relaxation energy. TiO_2 nanoparticle has low oxygen vacancy formation energy and narrow band gap by defect state, and can be utilized as an efficient photocatalyst material.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-378**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Characterization of Crystal Structure of Biodegradable Poly(3-hydroxybutyrate- co-3-hydroxyhexanoate) Blend with Polyethylene Glycol in Thin Films

<u>Yujing Chen</u> 박연주 Chunming Yang[1] Isao Noda[2] 정영미[*]

강원대학교 화학과 [1]2Shanghai Synchrotron Radiation facility, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, China [2]Department of Materials Science and Engineering, University of Delaware, MHG, Inc., USA

Understanding the crystal structure and thermal behavior of poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) (PHBHx) and its blends thin film under spatial confinement is crucial for its application in molecular scale devices and advanced nanotechnology. In this study, we investigate the influence of polyethylene glycol (PEG) on the morphology and molecular orientation of PHBHx thin films using scanning probe microscope and grazing-incidence wide-angle X-ray scattering. Unexpectedly, we found that addition of PEG actually increases the crystallinity of PHBHx and no hydrogen bonds were detectable in the thin film of PHBHx/PEG blend. PEG destroyed the edge-on lamellar orientation of PHBHx leading to the chain axis to pack preferentially in a direction between the out-of-plane and in-plane along with a flat surface. More importantly, analysis of the q space of (020) diffraction indicated that PHBHx crystal tends to form a densely packed lamellae after the addition of PEG. The thermal behaviors of such densely packed lamellae crystals were examined by temperature-dependent infrared-reflection absorbance spectroscopy and two-dimensional correlation analysis. It was revealed that the crystal structure of PHBHx/PEG blends were stable during the melting process despite the decrease of the crystallinity. We speculate that the reorientation and thermal stability of the crystalline PHBHx/PEG blends were due to PEG acting as an effective solvent that not only lowered the surface energy of chain folding surface but also changed the kinetics of PHBHx crystallization. Detail information will be discussed in the presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-379**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An Ingenious SERS Sensor for Glucose Detection Based on Enzyme Catalytic Reactions and Aggregation of Nanoparticles

FU CUICUI 진실아 오주희 정영미*

강원대학교 화학과

An ingenious and facile surface-enhanced Raman scattering (SERS) sensor based on the enzyme catalytic reaction and aggregation of silver nanoparticles (AgNPs) was designed for the determination of glucose. In this approach, 4-aminothiophenol molecules that were marked on the surface of AgNPs (AgNP@4-ATP) act as not only Raman tags but also linkage agents. When the AgNP@4-ATP was exposed to silver ions (Ag+) solution, an obvious SERS signal could be observed. We can trace the SERS intensity of 4-ATP to determine the concentration of glucose. This SERS biosensor has the potential of detection for clinical in the future.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-380**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel Design of Organic Dyes Based on Rigid Triphenylamine and N-Annulated Perylene for DSSC Application

ESTRELLA LIEZEL Mannix Balanay[1] 이상희 김동희[*]

군산대학교 화학과 [1]Department of Chemistry, Nazarbayev University, Kazakhstan

To cope with the unceasing increase of the global energy demand, considerable and extensive research efforts have been dedicated to the use of renewable energy resources, one of which is the utilization of the solar energy through photovoltaic devices. In line with this, research interests have been devoted to the design and synthesis of novel dyes with the goal of improving the efficiency of dye-sensitized solar cells (DSSCs). In this research, we introduce a group of metal-free dyes based on rigid triphenylamine donor group incorporated with N-annulated perylene as π-spacer. Density functional theory (DFT) and time-dependent DFT (TD-DFT) methodologies were utilized to investigate the geometry, electronic structure and UV-Vis absorption spectra of these dyes. The calculated results show that using rigid triphenylamine and N-annulated perylene provides broadened and bathochromically shifted absorption spectra. Furthermore, the calculated ground-state and excited-state oxidation potentials indicate that all of the dyes exhibit an efficient electron injection and dye-regeneration. The results obtained in this research will serve as a useful reference for the future dye designs for DSSC applications.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-381**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on the degradation mechanism of charged cathode surface using 2D correlation spectroscopy

김예슬 박연주 정영미[*]

강원대학교 화학과

Li-ion batteries are widely used in many portable electronic devices and are anticipated to be future energy storage devices. For these applications, it is essential to improve its capacity, power, durability, and safety. However, electrochemical reactions involved in the degradation process are very complicated and the full scenario of the relationship between the surface structural degradation and degradation of devices is still not well understood. In this study, the structural change of $LiCoO_2$ cathode during charging process are monitored by in-situ Raman spectroscopy. For better understanding the mechanism of the change of cathode materials, we also performed principle component analysis and 2D correlation spectroscopy. Details of degradation mechanism of charged cathode surface will be discussed in this presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-382**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation of Small Size Water Clusters of Superacidic Sulfur Oxoacids

정유경 김성규[1,*]

성균관대학교 기초과학 연구소 [1]성균관대학교 화학과

Van der Waals clusters of strong acids with water molecules may form dissociated structures as the number of hydrated water molecules increases over a certain threshold. Less water molecules are needed to dissociate strong acids. Recently, one of us reported that only two water molecules can dissociate disulfuric acid, which breaks the record of three water molecules that are needed to dissociate $HClO_4$ (S.K.Kim et al. Phys. Chem. Chem. Phys. 2015, 17, 28556). In this presentation, we report recent ab inito caculations for water clusters of superacidic sulfur oxoacids $H_2S_nO_6$ (n=2-4) to extend the study of dissociation phenomena in strong acid-water clusters.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-383**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Detection of toluene using a simple SERS substrate

오주희 진실아 박연주 정영미[*]

강원대학교 화학과

Detection of hydrophobic molecules, such as toluene, benzene, drugs has been widely studied. However it is still difficult to quickly and efficiently detect hydrophobic molecules. Surface–enhanced Raman Spectroscopy (SERS) is a powerful analytical technique for highly sensitive detection of molecules. In this study, to detect hydrophobic molecules based SERS, self-assembled bilayer cetyltrimethylammonium bromide (CTAB) on Au substrate was used. The interior of the self-assembled bilayer CTAB is highly hydrophobic molecules can thus be dissolved in this region. We observed that a simple SERS substrate using self-assembled bilayer of CTAB is useful to detect hydrophobic molecules. Details on the result of detecting toluene using this simple SERS substrate will be discussed in the presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-384**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Simple Detection Method of Chemical and Biological Weapons Based on SERS

진실아 오주희 박연주 **Lei Chen**[1] 정영미[*]

강원대학교 화학과 [1]Jilin Normal University

Recently, more sensitive, more cost-effective and simple detection of chemical and biological (CB) weapons is very important issue. Surface enhanced Raman Scattering (SERS) can provide rapid and ultrasensitive detection method with a large amount of fingerprint information for the identification of biological materials even chemical materials. In this study, we detected hydrazine and thiodiglycol as chemical weapons and Bacillus subtilis and Bacillus cereus as biological weapons by using SERS. Details on simple detection of CB materials by using SERS will be discussed in this presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-385**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Characterization of Terbium Dopped Gadolinium oxide Nanoparticles

SHANTI MARASINI 이강호*

경북대학교 화학과

It is known that lanthanide oxide nanoparticles have drawn tremendous attraction because of their strong paramagnetic and fluorescence properties which facilitate us to utilize these nanoparticles as a MRI contrasting agent. In the present study ultrasmall gadolinium oxide nanoparticles doped with terbium ions were synthesized by polyol route. The structural and optical properties of the D- glucuronic acid coated Tb3+:Gd2O3 nanoparticles were studied by XRD, FTIR, TGA, HRTEM and PL. Cubic shaped nanoparticles with a diameter of 1-3 nm were characterized. Terbium ion significantly influenced the fluorescence property of the particles. The main objective of this work is to functionalize these nanoparticles towards target-specific imaging as MRI contrasting agent.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-386**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of an optical sensor for selective metal ions detection

김태훈 정연기 이기환*

공주대학교 화학과

Recently, the design and development of selective optical receptors for metal ions has gained extensive attentions, as metal ions play an important role in a wide range of chemical and biological processes. Herein, the colorimetric sensing probe has been synthesized by the reaction of rhodamine B acid chloride with benzhydrazide under reflux with triethylamine in acetonitrile. The synthesis of probe was confirmed by 1H NMR, 13C NMR and mass spectrometric analysis. The sensor showed high selectivities toward Al^{3+}, Cr^{3+}, and Fe^{3+} ions over competitive ions (Cd^{2+}, Pb^{2+}, Zn^{2+}, Hg^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Mg^{2+}, Ag^{2+}, Mn^{2+}, Na^{+}, K^{+}, Li^{+}) in aqueous methanol (1:1, v/v). Interestingly, the 1:1 ligand-metal binding stoichiometry was found by the Job's curve employing the UV-Visible titration experiment.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-387**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The relaxometric properties of ultra small gadolinium oxide nanoparticles coated with various ligands

MiaoXu 이강호*

경북대학교 화학과

In the past few years, much effort have been made on investigation of several ligands which is water soluble, biocompatible and can give better water proton relaxation. It is necessary that for biomedical applications, surface-modification of the nanoparticles is essential because nanoparticles should be water-soluble and biocompatible. The goal of this work is to examine the effect of the surface coating of gadolinium oxide nanoparticles on the longitudinal relaxivity (r1) in aqueous suspensions. In this work, we used different water soluble and biocompatible ligand for the surface coating of the nanoparticles. We observe that two effects ligand size and ligand-chain hydrophilicity effects on the relaxometric. Properties of ultra small gadolinium oxide nanoparticles.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-388**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of bismuth oxide nanoparticles for CT contrast agent

ADIBEHALSADAT GHAZANFARI SEYEDHOSSEIN 이강호*

경북대학교 화학과

In this work we synthesis water soluble and biocompatible D-glucuronic acid coated bismuth oxide nanoparticles as a potential CT contrasting agent. All the synthesized metal oxide nanostructures were characterized by transmission electron microscopy,powder X-ray diffraction and IR spectroscopy .The characterization result shows that all the particles are monodispersed in size,shape and highly crystalline in nature. The structural, morphological, other properties, and their application are studied. The goal of this work is to examine the effect of the surface coating of bismuth oxide nanoparticles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-389**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Water Proton Relaxivity and Fluorescence Properties Study of Surface-Modified Gadolinium Europium Oxide ultrasmall Nanoparticles

Xu Wenlong 이강호*

경북대학교 화학과

We report the synthesis and the properties of surface-modified ultra-small europium mixed gadolinium oxide nanoparticles. It was characterized by XRD, FT-IR, TGA, HRTEM, Fluorescence spectrophotometer, and MRI instrument. The average particle diameter (davg) of the nanoparticles was estimated to be ~2 nm. The gadolinium europium oxide nanoparticles were found to be strong paramagnetic and emitted red fluorescence. The nanoparticles exhibited non-cytotoxicity up to 100• M concentration and showed the positive contrast-enhancement on mouse liver and kidneys after the injection of nanocolloid in vivo MRI. Hence, it can be used as a MR-Fluorescence imaging agent.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-390**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Conjugation of ultrasmall Gd2O3 nanoparticles with Trans-activator of transcription (TAT) peptide and its application in vitro and in vivo MR imaging

AHMAD MOHAMMAD YASEEN 이강호[1,*]

경북대학교 chemistry [1]경북대학교 화학과

We demonstrate a simple one-pot synthesis of TAT peptide-conjugated ultrasmall gadolinium oxide nanoparticles (Gd2O3). The sample was characterized by HRTEM, XRD and FTIR spectroscopy techniques. The conjugate had a mean particle diameter 1.6 nm. The relaxivity and in vitro cytotoxicity were investigated for potential application in magnetic resonance imaging (MRI). The r1 value of TAT-Gd2O3 NPs was measured to be Large r1= 18.2 s-1 mM which is higher than that of commercially available Gd-DTPA (4.57 s-1 mM). The aqueous sample (TAT-Gd2O3 NPs) is not toxic for the tested concentration range, however, toxicity increases with increasing concentration of Gd. These levels of cellular toxicity are sufficiently low to carry out in vivo MRI experiments. This study may provide an effective strategy for the design and development to target tumor cells.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-391**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Stability of CNT nanocontainers with high energy materials: reactive molecular dynamics calculations(고에너지물질을 충전한 CNT 나노컨테이너의 안정성: 반응성 분자동력학 계산)

조수경* 배광태[1]

국방과학연구소 4본부-2부 [1]국방과학연구소 4본부 2부

We have investigated chemical and thermal stabilities of CNT nanocontainers loaded with high energy materials (HEMs) by using reactive molecular dynamics (MD) calculations. The CNT containers and HEMs were built using Nanotube Builder and Amorphous Builder in MAPS 4.0 platform of Scienomics SARL. The reactive force field (ReaxFF) MD simulation was carried out by using the massively parallel LAMMPS package. The ReaxFF simulation used the NVE ensemble with RDX potential, which was known to provide excellent results for the reactions of HEMs. The simulation time was 50 ps, and the time step was 0.1 fs to investigate both chemical reactions of HEMs at high temperature and chemical stability of CNT containers.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-392**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photooxidation of Ternary Two-Dimensional Crystal $CrPS_4$

김수현 류순민*

POSTECH 화학과

그래핀과 MoS_2 로 대표되는 단원계 및 이원계 2 차원 결정에 이어 강자성 또는 반자성을 띄는 MAX_n (M=전이금속; A=P, Si, Ge; X=S, Se, Te; n=3, 4) 형태의 삼원계 2 차원 물질에 대한 관심이 증가하고 있다. 표면적이 극대화된 2 차원 물질의 화학반응은 3 차원 모물질과 다른 특이성을 보일 수 있으며, 광산화 반응 연구는 흡수된 빛 에너지의 흐름을 이해하여 광전 소자로의 응용 가능성을 타진하기 위해 필수적인 과정이다. 본 연구에서는 기계적 박리법을 이용하여 단일층 및 복층 $CrPS_4$ 를 분리하고, 라만 및 광발광 분광법을 이용하여 체계적으로 광산화 반응을 연구하였다. 비교 실험으로 수행된 고온 산화 반응에서는 MoS_2 와 유사한 수준의 역치 온도를 보인 반면, 레이저 광 조사 실험에서는 광열 반응 메커니즘이 확인된 MoS_2 에 비해 1/100 수준의 낮은 세기에서 산화되는 것을 확인하였다. 두 시료의 흡광 및 방열되는 정도가 비슷하다고 가정할 때, $CrPS_4$ 는 전자전이가 핵심적인 역할을 하는 광화학적 산화 반응을 따른다고 예상된다. 자세한 반응 메커니즘을 이해하기 위해 광자 에너지의 영향과 광조사에 의해 유발된 결정의 온도 변화를 분광학적 방법으로 측정하였다. 현재까지 2 차원 $CrPS_4$ 결정에 대한 연구는 전무하며, 2 차원 결정의 일반적인 광산화 메커니즘을 이해하기에는 기존에 수행된 연구가 충분하지 않다고 판단된다. 또한 산화 및 열화 현상을 이해하는 것은 반도체 및 광전 소자의 안정성을 향상시키기 위해 필수적이라는 점에서 이 연구는 큰 의미를 가진다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-393**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gd_2O_3 Nanoparticles Coated HA as Bimodality MRI Contrast Agent

HOSONLONG 이강호*

경북대학교 화학과

Recently, highly stable and highly biocompatible, low toxic nanoparticles that specifically target organs or cells are catching greater interest in nanobiology and medicinal chemistry. In another hand, hyaluronic acid (HA) is often used as a tumor marker for cancer, it can also be used to monitor the progression of the disease. This work describes the synthesis of Gd_2O_3 nanoparticles coated HA which were characterized by XRD, ICP-MS, TGA, FT-IR, TEM, relaxivity and can be used as cancer diagnose MR imaging contrast agent.References1.Philip S. Low, Walter A. Henne, and Derek D. Doorneweerd. “Discovery and Development of Folic-Acid-Based Receptor Targeting for Imaging and Therapy of Cancer and Inflammatory Diseases”. Accounts of Chemical Research 41, 120-129, 2009.2.Josefsson A., Adamo H., Hammarsten P., Granfors T., Stattin P., Egevad L., Laurent A.E., Wikström P., Bergh A. “Prostate cancer increases hyaluronan in surrounding nonmalignant stroma, and this response is associated with tumor growth and an unfavorable outcome” . American Journal of Pathology 179, 1961–1968, 2011 .3.Gritsenko P.G., Ilina O., Friedl P. "Interstitial guidance of cancer invasion". Journal of Pathology 226, 185–199, 2012.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-394**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The development of hyperspectral mid-IR high-resolution microscope

권혁상

한국표준과학연구원(KRISS) 미래융합기술본부/나노바이오측정센터

The study of biomolecules by IR spectroscopy has been carried out over the past decade with a strong correlation between the specific finger prints and various disease states in cell and tissue. The one of the attractive points of IR microscopy is the quantitative results based on the absorbance, in addition to non-destructive and label-free detection. However, it has not yet reached its potential for the highly selective and sensitive detection with a high resolution (~μm/point) imaging within a few minutes. Recently, we developed IR microscope based on a broadly tunable mid-IR quantum cascade laser (QCL, 5.5 ~ 12 μm). The QCL has a higher spectral radiance than FT-IR source (~10^6 times) and synchrotron source (~10^3 times), which makes much better signal to noise ratio. Our home-built IR microscope operates in LabVIEW based imaging and analysis programs. The performance test has been conducted with the resolving of a patterned organic thin-film and a 2D hyperspectral imaging for the finger prints of the selected mid-IR wavelength.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-395**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical infrared spectrum of a-type peptide ion derived from triglycine

임승택 신승구*

POSTECH 화학과

We present the infrared spectra of the transient species involved in unimolecular dissociation of the a-type fragment ion derived from the b2 ion of protonated triglycine. We calculated the microcanonical rate constant for every step of the reaction using RRKM theory based on the potential energy surface (PES), rotational constants and vibrational frequencies obtained from ab initio calculations. These PES and the molecular properties were calculated at B3LYP level of density functional theory with a 6-311++G(d,p) basis set. We examined the temporal variation of the population of the reactant, reaction intermediates and product by numerically solving the coupled differential rate equation using the matrix method. The temporal data were used to extract the rate constant for the overall reaction. Then, the infrared spectra of the a-type ion were calculated by taking into account the time-averaged population of reactant and reaction intermediates. The resulting infrared spectra of transient species were energy-dependent, and they showed no trace of the reactant. This result suggests that infrared spectra of dominent transient species provide fingerprints of reaction intermediates involved in a unimolecular dissociation reaction.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-396**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Two-Dimensional Tetracene Film Confined between Two Graphene Layers

구성현 류순민*

POSTECH 화학과

분자 크기의 공간에 속박된 분자는 자유 공간 또는 3 차원 응축상에 존재할 때와 다른 거동을 보인다고 알려져 있다. 이렇게 미시 세계에 속박된 분자를 재현성 있게 구현하는 일도 만만치 않은 일이지만 분광학적인 탐침과 호환성을 갖게 만드는 일은 더욱 어려운 일이 된다. 본 연구에서는 화학적 안정성과 높은 기계적 강도를 가지는 그래핀을 단일 분자층 속박을 위한 벽으로 활용할 수 있음을 확인하였다. 특히 그래핀은 98%에 가까운 높은 광학적 투과도를 가지고 있기 때문에 벽으로서의 역할 뿐만 아니라 ‘분광학적인 창’(spectroscopic window)으로서도 이상적인 물질이다. 먼저 기계적 박리법으로 만들어진 그래핀 위에 또 하나의 그래핀을 적층하는 ‘건식 미시 시료 전사법’을 최적화하여 그래핀/그래핀 적층 구조체를 형성하고, 라만 분광법과 원자힘 현미경을 이용하여 포집물이 최소화된 구조체의 특성을 분석하였다. 그래핀/분자/그래핀 샌드위치 형태를 구현하기 위해서는 바닥 그래핀 층 위에 1 nm 두께의 테트라센(tetracene)을 진공에서 증착한 후 상층 그래핀을 적층하였다. 속박된 분자는 증착 직후와 유사하게 평탄한 분자층을 이루고 있으나, 100 도 이하의 온도에서도 2 차원 공간을 통해 활발하게 이동한다는 사실을 알 수 있었다. 또한 속박된 분자층의 경우 광조사 대한 내성이 전반적으로 증가하여, 단분자층의 광발광 스펙트럼을 안정적으로 측정할 수 있었다. 본 연구에서 드러난 분자층의 형태와 광발광 스펙트럼의 특성은 속박된 분자의 거동 및 이차원 결정-분자 간의 상호작용을 이해하는 일에 단초를 제공할 것이다. 또한 본 연구는 광열화로 인해 분광학적인 연구가 용이하지 않은 물질에 대해서 안정적인 측정 환경을 제공할 수 있다는 점에서도 큰 의의를 갖는다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-397**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optical Second-Harmonic Generation from MoS$_2$/Al$_2$O$_3$/MoS$_2$ Heterostructure

김원택 류순민*

POSTECH 화학과

Optical second-harmonic generation (SHG) is a nonlinear optical phenomenon where two photons with same frequency produce a new photon with twice the energy. Since the first SHG-generation of UV light from a ruby laser beam in 1961, SHG has long been utilized in studying various non-centrosymmetric systems. However, it has not been experimentally explored how induced SH polarization field interact with another on a nanometer length scale. In this work, we investigated SHG from two parallel plane-confined polarization fields separated by a precisely controlled distance. Hetero-structures of MoS2/Al2O3/MoS2 serving as a model system was prepared by first growing an Al2O3 layer with a preset thickness defining the interlayer spacing on single-layer MoS2 by atomic layer deposition (ALD) and then precisely placing another single-layer MoS2 on top of the Al2O3/MoS2 stack. The azimuthal stacking angle between the two MoS2 layers were also controlled during the assembly. Polarization-resolved behavior and spacing-dependence of SHG will be discussed. In addition, details of the assembly process and structure of the heterostacks will be presented. This work will deepen our understanding of low-dimensional nonlinear optics.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-398**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A portable GC using ambient air as carrier gas for in situ monitoring of environmental pollutants

유동욱 정광우*

원광대학교 화학과

Current study describes a prototype of portable GC (30×20×15 cm3 and 5 kg) for real-time and quantitative determinations of gas mixtures in air sample. This system, powered by either a 24 V DC adapter or batteries, consists of a preconcentrator/injector, a 30-m capillary column with at-column heater configuration and a modified photoionization detector (PID). Ambient air is employed as a carrier gas, and a diaphragm pump is used to push the carrier gas. The analytical cycle including sampling, separation and cooling required less than 10 min. Optimum average flow velocity of carrier gases (air and He) were measured for best resolution of the system. The results indicate that this portable GC is expected to be used for a wide range of applications, particularly for in situ environmental monitoring, chemical processes, and regulation of contaminant emission.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-399**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Mixed DyEuO_3 Nanoparticles Coated D-Glucuronic Acid as Bimodal MR-Optical Imaging Agent

양병우 이강호[1,*]

경북대학교 응용화학과 [1]경북대학교 화학과

Herein, mixed DyEuO_3 nanoparticles coated D-Glucuronic acid were synthesized and characterized by XRD, HRTEM, FT-IR, Fluorescence spectrophotometer, TGA, SQUID magnetometer and MRI instrument. These nanoparticles had an average particle diameter of ~3 nm and monodisperse and emitted a strong blue fluorescence. Toxicity of these nanoparticles were also tested and showed non cytotoxic up to concentration of 500 μM. In vivo MR experiments on mouse liver and kidney showed negative contrast enhancement. Therefore, these nanoparticles can be used as bimodal MR-optical imaging agent.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-400**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular Design of Hole Transport Material for Perovskite Solar Cell through Bridge Modification of the Tetraphenyl Benzidine Based Molecules

GAPOL MAEBIENNE ANJELICA Mannix Balanay[1] 이상희 김동희*

군산대학교 화학과 [1]Nazarbayev University

Perovskite solar cell (PeSC) has risen as a new key competitor in the field of photovoltaic technology due to its highly progressive developments with a certified efficiency of 22.1%. Discovery of a novel hole transport material (HTM) in PeSC is a foremost area of research aiming to improve the performance and stability of the device. TPB linked to a carbazole moiety through a double bond has been used as a dopant-free HTM in PeSC and has yielded a comparable efficiency to the device using doped Spiro-OMeTAD. In this presentation, the modification of the bridge moiety between the TPB and carbazole was done. Energy levels, absorption spectra and electrochemical properties of the derivatives were investigated using the density functional theory and time-dependent density functional theory. Compared to the reference molecule, the derivative with thiophene linker produced a lower HOMO level and hole reorganization energy. Also, it has a blue-shifted absorption which is good for less competition with the perovskite visible light absorption. Thus, thiophene linked derivative is a promising HTM in PeSC.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-401**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solvolysis Mechanism Analysis of 4-Methoxyphenyl Chloroformate

이나경 박경호[1,*]

한양대학교 응용화학과 [1]한양대학교 과학기술대학 응용화학과

Solvolysis of 4-methoxyphenyl chloroformate (**1**) was performed in several pure and aqueous binary solvents at 25.0 ^{o}C. The conductivity method was applied in order to obtain rate constants appropriately, because **1** was predicted that it has fast reactions for solvolysis. These rate constants for each solvent system were analyzed by the extended Grunwald-Winstein equation primarily, additionally the activation parameters and kinetic solvent isotope effect. All results were indicated that **1** proceed through S_N1 reaction mechanism, specifically ionization pathway. This phenomenon is consistent with that of phenyl chloroformate (**2**) previously reported, **2** has Ionization pathway in all solvent. **1** has different a little with methoxy substituent at *para*-position. This methoxy group has an inductive effect to donate electron toward benzene ring structure. It is helpful to ionize the leaving group, Cl ion, from **1**. Also this effect is the reason that **1** has larger rate constants than **2**.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-402**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Stacking-specific infrared plasmons of trilayer graphene revealed by spectro-nanoscopy

최부건 정규일 이한결[1] 김지환[2,*]

서울대학교 화학부 [1]서울대학교 자연과학대학 화학부 [2]서울대학교 화학과

Trilayer graphene can have Bernal (ABA) and rhombohedral (ABC) stacking domains with distinct band-structures. Using the scattering-type scanning near-field optical microscopy (sSNOM), we investigated how such difference in band structures lead to different surface plasmon polaritons (SPPs) at infrared frequencies. The naturally doped ABA or ABC-stacked graphene on SiO2 substrate show sSNOM spectra of SiO2 phonon modes that are modified by the presence of the graphene. Furthermore, the spectral modification, which arise from the coupling between phonon of SiO2 and SPP of graphene, is found to be stacking-specific. The sSNOM images around ABA / ABC boundaries show strong reflection of SPPs at the boundaries, and such reflection is found to be dependent on the gating voltage applied to the substrate. Both of the data clearly show that the SPPs are different for ABA and ABC structures. We believe that the difference in SPP mode arise from the difference in intraband (Drude-type) conductivities for the two stacking domains. Such difference in optical conductivity is also determined by the band-structure and the degree of doping. The interpretation is fully supported by near-field tip-sample coupling model and tight-binding band structure calculation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-403**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

SERS monitoring of the photo-electrochemical reaction of 4-methylbenzenethiol on metallic surfaces

이강섭 최한규 신현항 박상민 연규진 김지환[1,*]

서울대학교 화학부 [1]서울대학교 화학과

We observed an unusual photo-electrochemical reaction of 4-methylbenzenethiol (MBT) on metallic surfaces. The potential-dependent surface-enhanced Raman scattering (SERS) spectra (λ_{ex} = 632.8 nm) and cyclic voltammetry (CV) were monitored from the junction of MBT-modified silver nanoparticles (AgNPs) dispersed on gold thin film (AuTF). When the potential is swept from -0.1 V to 0.3 V (anodic sweep), SERS spectra and background of MBT suddenly disappear, which is caused by oxidation of AgNPs. On the other hand, in the cathodic sweep (0.3 V to -0.1 V), we observed SERS spectra with 6 new peaks. We also found that the new SERS peaks are generated only when laser excitation and electrochemical potential are present. With the help of density functional theory (DFT) calculation, we attribute the new SERS peaks to 4-mercapto-3,5-dinitrotoluene, which is generated by aromatic substitution induced by metal-MBT charge transfer (CT).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-404**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Monitoring the initial reaction step in the photocatalytic reduction of nitrobenzenethiols using surface-enhanced Raman scattering

최한규 이강섭 신현항 김지환[1,*]

서울대학교 화학부 [1]서울대학교 화학과

Reduction of nitrobenzene is widely used as a model reaction for assessing the catalytic activities of nanoparticles, yet the detailed mechanism is still largely unverified. Here we have identified an intermediate of the first reaction step in the photo-catalytic reduction of nitrobenzenethiols (NBTs) on silver and gold using the time-resolved surface-enhanced Raman scattering (SERS). The formation of the intermediate is identified by a fast red-shift (with a time constant of ~1 sec) of the NO_2 symmetric stretching peak (ν_{NO}) of the SERS spectra of reacting NBTs, prior to a slow (~10 sec) intensity decay of the peak. Based on the laser power dependences of the rates of spectral changes, electrochemical SERS measurement, and quantum chemical calculations of the spectra, we conclude that the intermediate is the anion radical of nitrobenzenethiol or its conjugate acid, which is formed through the transfer of an electron from metallic surfaces. The subsequent slow intensity decay, which is the rate-determining step of the whole reaction, is another single-electron reduction of the anion radical into dihydroxyaminobenzenethiol or dianion of NBT. Our result disproves the usual assumption that apparent intensity decay rate of ν_{NO}–peak of nitrobenzene reflects the reduction kinetics of neutral nitrobenzene.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-405**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Generation of SERS hotspots with well-defined crystalline facets

이승연 구자정 김지환[1,*]

서울대학교 화학부 [1]서울대학교 화학과

The heterogeneity in surface-enhanced Raman Scattering (SERS) activities partly arise from the random crystalline facets of nanoparticles constituting the plasmonic gaps. To investigate such influence, we fabricated the SERS hotspots made of nanocube-molecule-nanoprism with well-defined {111}-facets. Single-crystalline gold nanoprisms that were synthesized with polydiallyldimethylammonium chroride (PDDA), lead to large, atomically flat surfaces with {111}-facets. Silver nanocubes that were synthesized have well-defined {111}-facets. The nanocube-methylbenzenethiol-nanoprsim junctions are self-assembled and SERS activities of each junction are measured. The SERS activities from such junctions are compared with usual polycrystalline plasmonic junctions with similar geometries.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-406**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Hot-electron mediated mode-specific vibrational excitation of molecules at a plasmonic gap

신현항 최한규 연규진 박상민 이강섭 김지환[1,*]

서울대학교 화학부 [1]서울대학교 화학과

We observed mode-specific vibrational excitation of organic molecules by gap plasmons. The junctions are made of Ag nanoparticle (AgNP, diameter : 80 nm) – organic molecule (biphenyl-1,4-dithiol) – Au thin film (AuTF, thickness : 10 nm) and the Stokes and anti-Stokes peaks of surface-enhanced Raman scattering are monitored. A focused laser illumination (λ_{ex} = 632.8 nm) of the junction shows an intermittent blinking (on and off) of ν = 1600 cm^{-1} (C-C stretching mode) anti-Stokes peaks whereas other equally strong peaks (ν = 1100 cm^{-1} and 1300 cm^{-1}) does not show any such blinking. The “off-state” spectra shows Stokes to anti-Stokes ratios that can be explained by optical Raman pumping effect. On the other hand, the unusual anti-Stokes to Stokes ratios for “on-state” is cannot be explained by such effects. Based on dark-field spectroscopy, density functional theory calculation and Frank-Condon analysis, we conclude such abnormal vibrational excitation arise from the interaction of molecules and the plasmonic hot electron tunneling between AgNP and AuTF.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-407**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparisons of *para*-Substituted Benzoyl Chloride Derivatives

김정은 박경호[1,*]

한양대학교 응용화학과 [1]한양대학교 과학기술대학 응용화학과

Benzoyl chloride derivatives have been studied analyses of mechanisms for solvolysis. Benzoyl chloride, one of the aryl halides, has very good structure to study the mechanism, S_N1 or S_N2, because it has carbonyl carbon as a reaction center, whose electron density is affected by a substituent on adjacent benzene ring. 4-Methoxybenzoyl chloride (**1**), 4-methylthiobenzoyl chloride (**2**), 4-trifluoromethoxybenzoyl chloride (**3**), and 4-trifluoromethylthiobenzoyl chloride (**4**) were compared with rate constants, and the results of Grunwald-Winstein equation analyses. All these substrates have a substituent on *para*-position, based on methoxy group, **2** has 4-methoxy group with sulfur instead of oxygen. **3** has three fluorine atoms instead of three hydrogens, **4** has a sulfur and three fluorine atoms. Sulfur has a weak inductive effect than oxygen to donate electron toward adjacent benzene ring, however fluorine atom has strong inductive effect than hydrogen with same way. These factors affect to the electron density on reaction center. This comparison will show how the reaction mechanism can be changed along the above effects.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-408**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Influence of nanometric molecular position on far-field SERS radiation profile

연규진 최한규 박상민 신현항 이강섭 김지환[1,*]

서울대학교 화학부 [1]서울대학교 화학과

In this study, we theoretically studied how a-few-nanometer displacement of a single Raman-emitting molecule in plasmonic nanogap will be observed in the SERS radiation pattern in far-field region. We performed finite-difference time-domain (FDTD) simulation to calculate the far-field SERS radiation profile of a single Raman-emitting molecule located at a nano-sized gap of Ag nanoparticle dimer as a function of molecular displacement from the hotspot center. We found that an angular distribution of the far-field radiation become asymmetric and the corresponding real space image is also displaced when the molecule moves away from the hotspot center. We conclude that just a few-nanometer change in the molecular location in hot spot area can be sensitively detected in far-field region, which explains the recent experimental report on super-resolution mapping of the SERS hotspot.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-409**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photocatalytic CO2 Reduction by Copper(Ⅰ) Iron Oxide(CuFeO2)/Copper(Ⅱ) Oxide(CuO)/Reduced Graphene Oxide(rGO)/Polypyrrole(PPy) Cathode

정혜영 강영수*

서강대학교 화학과

Photocatalytic CO2 reduction for the production of hydrocarbon compounds is one of the most important strategies to decrease the atmospheric CO2 level and obtain the valuable hydrocarbon fuels, which can solve global warming and fossil fuel energy resource depletion simultaneously. Our research group has constructed CO2 reduction devices with semiconductor/rGO material, and investigated CO2 conversion using CuFeO2/CuO/rGO/PPy photocathode fabricated via electrodeposition. Both CuFeO2 and CuO are p-type semiconductors, and rGO has a large electrical conductivity to do multi-electron shuttling function from the conduction band of CuO to the CO2 molecules adsorbed on the surface of rGO. In addition, PPy is conducting polymer and has an ability to have lower activation energy for the CO2 reduction reaction. We fabricated the advanced type of cathode by electrodeposition of mixed rGO/PPy onto bare CuFeO2/CuO. PPy can increase the mechanical stability of the rGO with strong interfacial contact and it has also been reported as electrocatalysts for CO2 conversion with lower overpotential than metals. The hybrid material can improve the photocatalytic activity, and produce liquid fuel selectively with synergetic effect of CuFeO2 , CuO, rGO, and PPy.[1] Kang, U. S.; Choi, S. K.; Ham, D. J.; Ji, S. M.; Choi, S. M.; Choi, W. Y.; Han, D. S.; Abdel-Wahab, A.; Park, H. W. Energy Environ. Sci. 2015, 8, 2638[2] Won, D. H.; Chung, J. H.; Park, S. H.; Kim, E. H.; Woo, S. I. J. Mater. Chem. A 2015, 3, 1089[3] Kim,C.W.; Son,Y.S; Kang, M.J.; Kim, D.Y.; Kang,Y.S. Adv. Energy Mater 2015, 1501754

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-410**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A simple rhodamine B-based colorimetric sensor for selective detection of metal ions

전우주 정연기 이기환*

공주대학교 화학과

In recent years, selective optical receptors for the detection of environmentally and biologically important metal cations have received extensive attention for designing and development of colorimetric chemosensors. Herein, we report the rhodamine B-based colorimetric sensing probe for selective metal ions detection in the organic or mixed aqueous-organic media at neutral pH under ambient condition. The structures of synthesized compounds were characterized by IR, 1H NMR, 13C NMR and mass spectra. The 1:1 ligand-metal binding stoichiometry was found by the Job’s curve employing the UV-Visible titration experiment. The limit of detection and the association constant between the receptor and metal ion were confirmed by the 3σ slope-1 and Benesi-Hilderbrand relation, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-411**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Spectroscopic Approach to Photo Oxidized Degradation Process of PTB7 polymer

안규상 김봉수[1] 이경구[2] 곽경원[*]

고려대학교 화학과 [1]이화여자대학교 사범대학 과학교육과 [2]군산대학교 화학과

There have been numerous efforts to make portable and/or wearable Organic Photovoltaic(OPV) devices. Owing to its flexibility and small weight. The main hurdle in making such devices is the stability of the OPV donor material which get decomposed in presence of oxygen and light, hence decreasing the operational life time of the device. To improve its stability, various approaches have been followed such as better sealants and coating to minimize the passage of oxygen & water vapor into the device, development of scavenger which targets the species harmful to the device, better optical coating and design. Our purpose is the chemical modification of the OPV donor material. First, we checked the photo-degradation mechanism of well-known OPV material, PTB7 polymer by FT-IR measurement. Then, we use DFT calculation to get vibrational frequencies of the proposed intermediates. To trace a photochemical degradation mechanism, we compared the experimental and the computational IR value. To have better insight, we plan to build a Raman spectroscopy in house to use the Raman active C=C vibration to understand the photo-degradation process. Our findings will help in designing better OPVs by choosing the modified donor material.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-412**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Configuration study on the binary solvent mixture: MeOH-AcOH system

권영민 김찬경[1,*]

인하대학교 화학화공공학융합학과 화학전공 [1]인하대학교 화학과

In a pure solvent, a number of small clusters formed in the liquid. When two solvents are mixed together in a binary solvent, the number of homo- and hetero-clusters increases rapidly. In particular, the clusters of solvent molecules can influence various physical and chemical properties of the solvent. The structures of the clusters are quite diverse and not defined well in numerous solvents. In this work, several clusters in the methanol-acetic acid binary system were studied using the B3LYP/6-31+G(d) level of theory. Especially, we calculated all the possible isomers of homo-dimers and -trimers of methanol and acetic acid, respectively and hetero dimers and trimers of methanol-acetic acid mixture. All calculations were performed by Gaussian 09 package.

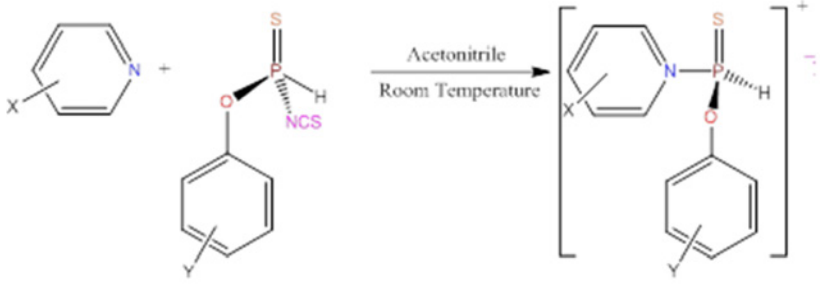
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-413**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical Studies on Nucleophilic Substitution Reactions of Phenyl Thiophosphonyl Isothiocyante with Pyridines Through Frontal Approach

Adhikary Keshab Kumar 김찬경*

인하대학교 화학과

We have studied phosphoryl and phosphonyl transfer reactions with pyridines, anilines and benzylamins. The phosphoryl transfer systems are proceeded either through concerted or stepwise pathway. There are many examples in the literatures where mechanistic changeover is taking place during the process. Our present study focuses on the mutual interaction of the substituents in the nucleophile and substrate, energy correlation analysis and the cross interaction constant4 (CIC), ρ_{XY}. In this work, the reaction mechanism for the pyridinolysis of phenyl thiophosphonyl isothiocyanates are investigated using the CPCM approach in acetonitrile at the B3LYP/6-311+G(d,p) level of theory. We optimized all the reactant complexes, transition states, and product complexes to obtain the potential energy surfaces for seven different substituents of X and Y for nucleophiles and substrates, respectively. Frequency calculations were performed to confirm the stationary species and to provide thermodynamic properties. The reaction mechanism is discussed in terms of Hammett reaction constants, ρ_X, ρ_Y, and cross interaction constant ρ_{XY} and the structure-energy relationships.



X and Y Substituents:
X = 4-MeO, 4-Me, 3-Me, H, 4-Cl, 3-Cl and 4-CN
Y = 4-MeO, 4-Me, 3-Me, H, 4-Cl, 3-Cl and 4-CN

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-414**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photochemical solar fuel production via CO2 conversion performing on the ZnTe/r-GO/PPy/Nafion photocathode

김소연 강영수*

서강대학교 화학과

The excessive utilization of fossil fuels is accompanied by large amounts of anthropogenic CO2 emissions, leading to adverse global environmental changes. Since solar power is a theoretically infinite energy source, the solar-driven reduction of CO2 into chemical fuels such as formic acid, methane or methanol has been considered as a promising approach to address the problems of global warming and energy crisis. Zinc telluride, ZnTe, is one of the most promising semiconductor photocatalyst which could conduct CO2 conversion to provide solar fuel by combing with r-GO, polypyrrole (PPy) and Nafion. It has been recently highlighted because its large negative energy value of conduction band edge (-1.63 V versus the reversible hydrogen electrode (RHE)) with a direct band gap of 2.26 eV shows the high capability of reducing CO2 to highly reduced liquid product. Also ZnTe have been used for the visible-light induced ($\lambda \geq$ 420nm) photoreduction of CO2. Synthesizing ZnTe nanoparticle based on the chemical replacement reaction between metal ions(Zn2+) and chalcogenide ions(Te2-). ZnTe photocathode shows efficient results of artificial photosynthesis. The prepared ZnTe particle layer will be coated with PVP and Nafion to have lower activation energy and one-pot reaction media, respectively, during CO2 reduction reaction. r-GO has a large electrical conductivity to do multi-electron shuttling function from the conduction band of ZnTe to the CO2 molecules adsorbed on the surface of rGO. In addition, Nafion has proton conductivity from outer layer of cathode to inner layer to do one-pot reaction to produce liquid solar fuels. PPy is conducting polymer and has an ability to do CO2 activation to get higher reactant energy levels to have lower activation energy for the CO2 reduction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-415**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photocatalytic CO2 Reduction by Z-scheme Photocatalytic Mechanism of WO3/g-C3N4/PVP/Nafion Electrode System

최보경 강영수*

서강대학교 화학과

CO2 is one of the major contributors to the global warming caused by fossil resource depletion. Therefore, it needs to develop a clean, renewable, cheap and sustainable source of energy to replace fossil fuels and meet the increased energy demand. So we need to develop methods to induce photocatalytic CO2 reduction to produce hydrocarbon fuels under solar light irradiation. Due to its high stability and narrow band gap, g-C3N4 is novel, nonmetallic semiconductor. WO3 is also a visible light responsive photocatalyst with narrow band-gap energy (2.4 - 2.8 eV). Therefore, our research group has constructed CO2 reduction reaction system with Z-scheme photocatalytic mechanism of g-C3N4/WO3. g-C3N4 will be prepared by using melamine in muffle furnace. 10 g of melamine will put into an alumina crucible with a cover and be heated at a rate of 2 °C min-1 to 550 °C in a muffle furnace and then keep at this temperature for 4 h. The synthesis of WO3 will be done as 1.0314 g NaWO4 and 0.3714 g of NaCl dissolved in 2 mL of 2 M HCl solution and stirred for 30 min. During stirring, 23 mL of distilled water will be added. The prepared g-C3N4/WO3 will be coated with PVP and Nafion to have lower activation energy and one-pot reaction media, respectively, during CO2 reduction reaction.[1] Chen, L.; Ma, W.; Dai, J.; Zhao, J.; Li, C.; Yan, Y. Journal of Photochemistry and Photobiology A: Chemistry 328 2016, 24–32[2] Aslam, I.; Cao, C.; Tanveer, M.; Khan, W.S.; Tahir, M.; Abid, M.; Idrees, F.; Butt, F.K.; Ali Z.; Mahmood, N. New J. Chem., 2014, 38, 5462[3] Kim, C.W.; Son, Y.S; Kang, M.J.; Kim, D.Y.; Kang, Y.S. Adv. Energy Mater 2015, 1501754

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-416**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced Photoelectrochemical Properties of (040) Crystal Facet Engineered BiVO4 Photoanode

지소현 강영수*

서강대학교 화학과

Artificial photosynthesis is generating solar chemical fuels by using incident solar-to-energy using semiconductor cell which has the cathode and the anode. When external solar energy which correspond to band gap of the material is irradiated, the electrons from balance band can be jumped up to conduction band. This excited electron can reduce the carbon dioxide molecule to hydrocarbon fuels by transporting to cathode part. For here, to reduce the carbon dioxide, protons and electrons have to be supplied at the same time. Anode parts carry out these taskHere, (040) crystal facet controlled BiVO4 is used for anode parts. Bismuth vanadate has many advantages for water oxidation. First, it has suitable bandgap for visible light response. Frequency of IR wave is low, so it doesn’t have enough energy for water splitting. Although UV light has sufficient energy but it’s portion is less than 5% in sunlight. And effective mass of charge carrier is lighter than other semiconductors. Additionally it is non-toxic, and has low photo-corrosion property, Composed of inexpensive elements. But experimental data value can’t reaches to theoretical one because of its several limiting factors like High recombination probability of photo-generated electron-hole pair and slow hole transfer kinetics for water oxidation. To overcome these limitations, method of crystal facet engineering has been tried. Because the exposed atoms on surface are altered depending on the morphology of semiconductor, it influences on photocatalytic performance of the material. By controlling crystal facet of BiVO4, despite of its constant light absorbing ability, photocatalytic properties are enhanced remarkably compared with uncontrolled BiVO4. This enhancement is come from increased conductivity of (040) crystal facet engineered BiVO4 . This (040) crystal engineered BiVO4 was synthesized by using hydrothermal method. [1] Kim, C. W.; Son, Y. S.; Kang, M. J.; Kim, D. Y.; Kang, Y. S. Adv. Energy Mater 2015, 1501754[2] Zhang, G.; Huang, C.; Wang X. Materials Views 2015, 9, 1215-1221

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-417**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A highly sensitive and selective fluorescent sensor for detection of mercury ion in aqueous solution at neutral pH condition

함현식 이기환*

공주대학교 화학과

A 3-(-4-metoxybenzol)-N-phenyl hydrazine carbothioamide(4) fluorescent sensor for highly sensitive and selective detection of mercury ion has been studied. The fluorescent sensor(4) after binding to Hg2+ion in pH7.00 buffered solution showed an increase in fluorescent emission intensity while a decrease in absorption intensity.Interestingly, the isosbestic point at 300nm in the probe upon successive mercury in addition gives solid evidence about the complexation between the probe and mercury ion. The 1:1 ligand-metal binding stoichiometry was assessed by an optical response experiment. The association constant and the detection limits the ligand toward Hg2+ ion were calculated to be 2.36 x 10-8M, 2.75 x 10-8M-1, respectively, employing the 3σslope-1method and Benesi-Hilderbrand equation. Also, the sensor showed high selectivity toward Hg2+ion over competitive ions (Fe2+, Cu2+, In3+, Mg2+, Al3+, Zn2+, Li+, Na+, K+, Ca2+, Sn2+, Si2+, Pb2+) in aqueous solution. The proposed sensing method might be a practical device for environmental samples analysis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-418**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of UV- curable fluorinated epoxy acrylate films with novel structures for hydrophobicity

이예정 김세아 김명화[1,*]

이화여자대학교 화학나노과학과 [1] 이화여자대학교 화학 나노과학과

We present the first synthesis of fluorinated epoxy acrylate (FEA) with isophorone diisocyanate (IPDI), diglycerol diacrylate (DGDA) and novel structure of fluorinated alcohol (F-ol), which was prepared based on hexafluoro benzene and fluorinated diol via Williamson ether synthesis. The newly prepared fluorinated urethane epoxy acrylate was carefully characterized with 1H-NMR & 19F-NMR spectroscopy and Fourier Transform Infrared (FT-IR) spectroscopy. The UV-curable fluorinated epoxy acrylate was formulated by urethane acrylate oligomer, Ebecryl 1290, the obtained novel fluorinated urethane acrylate and photoiniator, 1-hydroxycyclohexyl phenyl ketone. The mixed composite of substances were coated between cover glassed and cured. Thermal analysis was performed by differential scanning calorimetry (DSC). Furthermore contact angle measurements of water against films of coatings were evaluated and have shown the hydrophobicity of the new fluorinated urethane acrylate.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-419**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Quantitative structure-property relationship for predicting the vapor pressure of organic compounds at different temperatures

백영란 김현정 이성광*

한남대학교 화학과

Vapor pressure (VP) is a key physicochemical property determining the partitioning behavior of a chemical between water, air, and soil. Therefore, VP is used to assess the ability of a chemical to partition into the gas phase and to assess the potential of a chemical for long-range transport to remote locations via the atmosphere. VP depends strongly on temperature and VP at different temperatures is important environmentally because it changes depending on the latitude or the season changes. Thus, it is necessary to predict the vapor pressure by including different temperature as important environmental factors. In this study, quantitative structure-property relationship(QSPR) model was developed to predict the solid vapor pressure and liquid vapor pressure of organic compounds at different temperatures. The molecular descriptors were calculated by PreADMET program. Multiple linear regression(MLR), support vector machine(SVM) were applied for prediction of VP at different temperatures. All models were developed and validated for bootstrap method and y-scrambling method. We also defined applicability domain for each of the models to set the reliable prediction range.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-420**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Prediction of the flammability limit of organic chemicals based on quantitative structure-property relationship study

이수정 김현정 이성광*

한남대학교 화학과

Flammability limits, which is usually in percentage volume (vol %) at 298K, is defined as the range of fuel concentration within which an explosive reaction is possible when an external ignition source is introduced. The lower flammability limit (LFL) is the minimum concentration, the upper flammability limit (UFL) is the maximum concentration in this concentration range. The flammability limit is important parameter for maximizing the stability in the chemical industry because it caused an explosion and fire flammable compounds. Recently, it is need to provide flammable information of new compounds because the new compounds being developed on the whole industry will increase more and more. In this study, quantitative structure-property relationship models were developed for predicting flammability limit of organic compounds from 2D chemical structure. Multiple linear regression and support vector machine are used to select best subset of descriptors related to flammability limit. And we confirmed the reliability and predictability in our models by performing y-scrambling and cross-validation. Finally, definition of the applicability domain of models could be used to specify the scope of the models. The results show that these models can be used to predict the flammability limit of a wide range of organic compounds.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-421**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of on-line management and properties prediction system for high-energy molecules(HEMs)

이승규 박한웅 서현일[1] 이성광[*]

한남대학교 화학과 [1]주식회사 퀀텀소프트 본사

The On-line management and properties prediction system for high energy molecules(HEMs) was developed as a tool of finding HEMs structure and estimating the HEMs properties. The system was implemented in JAVA and JSP and consist of three part. Firstly, PostgreSQL database used for data storage was applied to search and manage the diverse fields of HEMs (approximately 6000 high energy molecule). Additionally, we used PostgreSQL Cartridge of Chemaxon in DBMS for deploying chemical database management and search engine. Secondly, the prediction module l which can predict important HEMs properties such as impact sensitivity, heat of formation, crystal density and physicochemical properties such as molecular weight, formula, number of rotatable bond, pKa, logP, logD was integrated in this system. HEMs properties were predicted by QSPR(Quantitative structure property relationship), group additivity method and JChem library. Thirdly, the program provide the plot of HEMs performance and sensitivity to design new promising HEMs through enumeration of virtual compounds in Marvinsketch. The program is powered by linux computer with Apache web servers and Tomcat servlet containers installed. The developed system are expected to be very helpful and pioneering tools as well as to design new promising HEMs to many researchers in diverse chemical fields.Availability: the program is available on http://aci.hannam.ac.kr/mshems

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-422**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Proficient synthesis of highly crystallized Iridium dioxide (IrO2) nanorods for a variety application

김성실 정혜승 김명화[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

Highly crystallized Iridium dioxide (IrO2) nanorods were successfully fabricated with the usage of controlled pH with further heating and annealing. With the simple process to synthesize with no defect, the morphology and crystal structure of the samples were carefully characterized with field emission scanning electron microscope (FE-SEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD) Raman spectra, and high resolution transmission electron microscopy (HR-TEM). Results demonstrate that highly sufficient one-dimensional IrO2 nano-crystal structure was uniformly grown with highly dense dispersion. Furthermore, it could be extended and corporated with other nanostructured wires or fibers such as TiO2 nanofibers. Thus, it is looking forward to be applied to electrochemical catalysts since Iridium dioxide is commonly known for its good efficiency.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-423**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, Properties, and Applications of Polyethylenimine-Stabilized Silver Core/Gold Shell Nanoparticles

김인현 이건희[1] 김주원[1] 신익수[1,*] 신권수[1,*]

한국기초과학지원연구원 질량분석장비개발팀, 숭실대학교 화학과 [1]숭실대학교 화학과

Abstract: In this study, the silver core/gold shell nanoparticles (Ag@Au NPs) with controlled shell thickness have been synthesized using polyethylenimine (PEI) polymer as reducing and capping agent in aqueous solution. First, Ag nanoparticles were prepared by the reduction of AgNO3 with PEI and were used as cores. Then the thickness of Au shell was readily controlled by changing the Au3+ ion concentration of precursor. The as-prepared Ag@Au NPs showed good stability in H2O2 solution. The Au shell deposition on Ag core was clearly identified via transmission electron microscopy and energy dispersive X-ray spectroscopy. The surface-enhanced Raman scattering (SERS) characteristics of Ag@Au NPs were examined in detail. In this approach, the core Ag was found to provide the enhanced SERS activity while the Au shell provided the stability (resistance to oxidation, etc.) of nanostructure. In addition, the Ag@Au NPs prepared in this work have also been exploited as solid phase catalyst for the reduction of 4-nitrophenol to 4-aminophenol in the presence of NaBH4.References K. Kim, H. B. Lee, J. W. Lee, H. K. Park, K. S. Shin, Langmuir 2008, 24, 7178-7183.K. S. Shin, J. H. Kim, Bull. Korean Chem. Soc. 2011, 32, 2469-2472.P. P. Patra, G. V. P. Kumar, J. Phys. Chem. Lett. 2013, 4, 1167-1171.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-424**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of optical chemosensor for selective metal ions detection

성은아 정연기 이기환*

공주대학교 화학과

Recently, there has been significant interest in the design and development of optical chemosensor for recognition of environmentally and biologically important analytes with high selectivity, sensitivity and low detection limit. Herein, a novel colorimetric sensing probe for the multi selective detection of metal ions has been synthesized by the reaction of rhodamine B acid chloride with 2-fluorobenzoic acid hydrazide under reflux with triethylamine in acetonitrile. The sensor showed high selectivity toward Sn2+, Fe3+, and Cu2+ ions over competitive ions (Cr3+, Cd2+, Pb2+, Zn2+, Hg2+, Co2+, Ni2+, Ca2+, Mg2+, Ag2+, Mn2+, Na+, K+, Li+) in aqueous methanol (1:1, v/v). Interestingly, the isosbestic point at 326 nm in the probe upon successive tin ion addition gives the solid evidence about the complexation between the probe and tin ion. The iron and copper ions were similar with this case except for the different isosbestic points. The minimum detection ability of ligand toward tin, iron, copper ions were calculated employing the absorption titration experimental results which comes to be 1.52 x 10-6 M, 4.10 x 10-6M, 1.39 x 10-6M, respectively, and the association constant of tin, iron, and copper ions were obtained 1.28 x 10-3 M-1, 5.03 x 10-3 M-1, 4.57 x 10-4 M-1, respectively, by using Benesi-Hidebrand relation. The synthesis of probe was confirmed by 1H NMR, 13C NMR and mass spectrometric analysis.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-425**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Surface Passivation of InPZnS and InPZnS/ZnS Core/Shell Nanocrystals

정화준 김영수 임승택 신승구*

POSTECH 화학과

We observed the effects of surface passivation on optical properties of InPZnS and InPZnS/ZnS core/shell nanocrystals (NCs). InPZnS NCs obtained from Ecoflux were coated with one-monolayer ZnS shell. The InPZnS and InPZnS/ZnS NCs were passivated with metal- and chalcogen-binding ligand in toluene or in chloroform at room temperature. Their optical properties were monitored by both UV/visible spectrometer and fluorometer. The addition of both metal-binding ligand (MBL) and chalcogen-binding ligand (CBL) increased the photoluminescence intensity of the InPZnS NCs. The ZnS shell helps retain the optical properties of core InPZnS NCs in the presence of air. The results suggest that the MBL + CBL ligand system plays an important role in passivating surface traps on InPZnS NCs.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-426**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Studies on bimetallic catalytic nanoclusters

Nasir Shahzad 김찬경[1,*]

인하대학교 화학화공공학융합학과 화학전공 [1]인하대학교 화학과

High-performance electro-catalysts with excellent catalytic activity and long durability compared to Pt are urgently necessary for the fast development of energy storage and conversion systems. Bimetallic nanoclusters are well known for their unique and unexpected behaviors. Different bimetallic nanoclusters of platinum have been investigated for oxidation reduction reaction. Nonetheless, many mismatches were found in electrolytic trend even when the clusters with the same composition, shape and size were used. Many of this is responsible for the reaction conditions. However, one of the most important factor was ignored: how the relative positions of joining metal atoms within the cluster affect the catalytic properties. Studying the isomerism experimentally at the nanoscale is a hard task. Our quantum chemical calculations showed that the homotops of the cluster can greatly change the catalytic properties. From this, it is possible to design a nanocluster with proper composition, size and shape. It is also found that homotopy of the cluster is also vital for precise estimation of catalytic properties.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-427**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Color tune of NaYF4:Yb,Er Upconversion substrate according to the post-treatment

임수영 박찬량[1,*] 김형민[*] 민경률

국민대학교 생명나노화학과 [1]국민대학교 화학과

Some of the rare earth metal elements are a feature that has an optical phenomenon called upconversion (Upconversion; UC). UC is a phenomenon that the two or more photons are absorbed in excited state and emit light of lower wavelength than incident light through UC process. The progression route of UC phenomenon is divided into ESA (Excited-State Absorption) and ETU (Energy Transfer Upconversion). ESA is a phenomenon that photon is again absorbed from the excited-state of energy level of the rare earth metal, and ETU (Energy Transfer Upconversion) is a phenomenon that one atom in excited-state transfers to the excited state of other atoms. Using these features, solar cells, displays and the development of lasers, have been used in a variety of optical industry. Recently, photographed bio image using UNCP (upconversion nano particle; UNCP) has been utilized in biology, medicine, diagnostics, biological optical science. If the information is got through the image shooting of the luminous object, the luminous object with a lot of colors may include a variety of information than the monochromatic luminous object. Thus, in recent studies, Researchers attempted to synthesize UCNP of the various colors utilizing the color variation of the luminescence in accordance with the size and shape of UCNP. There are two major ways In order to get the luminescence of various colors. First, there is a method to synthesize by changing the ratio of the rare earth metal. Second, there is a method to mix the various UC materials. The color adjustment of the existing method is time consuming and has a disadvantage that it synthesizes each time in order to create the desired color. To overcome these problems, UC substance with a single color was produced on a thin substrate by introducing the method of Pulsed Laser Deposition (PLD). Unlike the existing method, the adjustment of the luminescence color of the substrate was obtained progressing post-treatment after the deposition. Starting with green, yellow, orange, to red, it was possible to adjust the various colors and this was found to be a result generated by non-radiative transition of Er3+ ion by OH.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-428**

발표분야: 물리화학

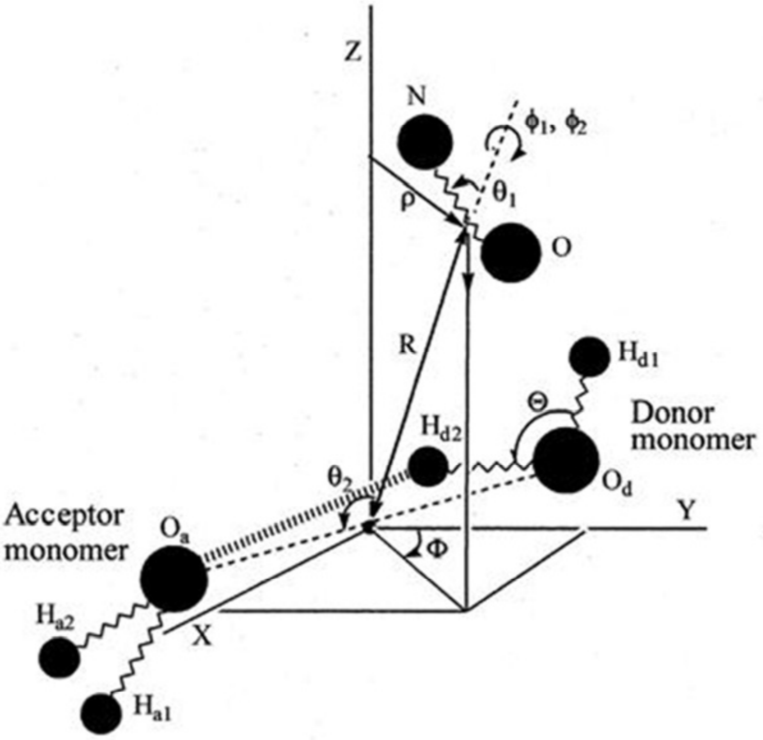
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dynamics of the Water Dimer + Nitric Oxide Collision

이종백* 김유항[1] **Hyung Kyu Shin**[2]

전남대학교 화학교육과 [1]한국과학기술한림원 [2]University of Nevada, Reno, NV

Collision-induced intermolecular energy transfer and intramolecular vibrational energy redistribution in the collision of a water dimer and nitric oxide. The energy gained by the dimer redistributes among various internal motions of the collision system, with the majority depositing in the H_2O stretches through the 1:1 resonance followed by the bend through the 1:2 resonance. Energy transfer from NO to the dimer is more efficient than that from the dimer to NO, the efficient attributed to internal modes operating as energy reservoirs. Strong long-range attractive forces are shown to contribute to the efficiency. The hydrogen bond shares about 10 % of the initial excitation stored in NO. A small fraction of the trajectories sampled lead to the hydrogen bond dissociation. The translational and rotational motions share the remaining energy. A small, but not negligible number of trajectories lead to binding of NO to the donor monomer.



Z
N
ϕ_1, ϕ_2
θ_1
ρ
O
R
H_{d1}
Θ
Donor monomer
H_{d2}
O_d
θ_2
Y
Acceptor monomer
O_a
Φ
H_{a2}
X
H_{a1}

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-429**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Crystallography of aligned hybrid perovskite single crystal arrays

__이린__ 성명모*

한양대학교 화학과

Lead halide perovskites CH3NH3PbX3 (X=Cl, Br, I) have received great attention because of their excellent photoelectronic properties as well as their low-cost device fabrication process. As an example, their theoretical efficiency limit of the solar cell devices was predicted around 31% by a detailed balance model for the reason that exceptional light-harvesting and superior carrier transport properties. Additionally, these excellent properties contribute to the applications of optoelectronic devices such as LASERs, LEDs, and photodetectors. Typically, one of the most important factor to decide the efficiency of these applications is the quality of the crystal. Even though, optoelectrical devices are composed of polycrystalline thin film in general, not a single crystalline form which has longer carrier diffusion length and lower trap density. For these reasons, perovskite single crystals have potential to elicit an optimized device efficiency.In this study, we analyzed the crystallography of the aligned perovskite single crystal arrays by X-ray diffraction (XRD) and selected area electron diffraction (SAED). Also the basic optic properties of perovskites were checked using optical mocriscope (OM) and scanning electron microscopy (SEM). From this work, the perovskite which is aligned in all directions both of out-of-plane and in-plane was fabricated and analyzed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-430**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of ZnO@SiO$_2$ core shell nanoparticles and its antibactrial activities

이유로 김우석 이얼 정동기 유정열 김재욱 김종규*

단국대학교 화학과

The ZnO@SiO$_2$ nanoparticles(NPs) in the form of quantum dots(QDs) have been synthesized in SiO$_2$ putting first or later in ethanol solution to form ZnO@SiO$_2$ NPs.The method of tetraethyl orthosilicate(TEOS) to an ethanol of ZnO nanoparticles produces random dispersion. The ZnO@SiO$_2$ NPs were examined by X-ray differaction spectroscopy(XRD), Scanning electron microscopy(SEM), Transmission electron microscopy(TEM) and antibactrial activity for *Escherichia coli* and *Staphylococcus auraus*. ZnO@SiO$_2$ NPs morphology show through X-ray differaction spectroscopy. Scanning electron microscopy(SEM) shows ZnO@SiO$_2$ morphological characteristics. Transmission electron microscopy(TEM) shows the lattice fringes corresponding to the (100) plane of the wurtzite ZnO structure. The antibactrial activities of ZnO@SiO$_2$ NPs show *E.coli* and *S.auraus*

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-431**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Heterojunction strain sensor with organic single crystal nanowire by direct printing

박윤경 성명모*

한양대학교 화학과

We fabricate organic single crystal nanowire heterojunction p-n diode with poly(3-hexylthiophene)(P3HT) and N,N′-Dioctyl-3,4,9,10-perylenedicarboximide (PTCDI-C8) using by liquid-bridge mediated nanotransfer molding(LB-nTM) method. LB-nTM has been reported an one step direct printing method for making well-aligned nanowire arrays. Moreover, multi-layering nanostructures can be fabricated with the consecutive printing process. As a result, it is possible to make simple and basic concept of heterojunction devices such as hetero p-n nanojunction diode. P3HT/PTCDI-C8 nanowires heterojunction diode has rectifying behavior with on/off ratios of ~10. Also it shows strain sensor properties also with external strain such as action of finger.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-432**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

ProWaVE: Protein Surrounding Water Visualization and Energetics

임해리 조한울 함시현*

숙명여자대학교 화학과

생체 내에서 일어나는 단백질의 구조와 기능을 이해하는데 단백질의 solvation thermodynamic 를 구현하고 이해하는 것은 매우 중요한 부분이다. 이를 위해 본 연구실에서는 www.prowave.org website 를 개발하였다. 본 website 는 누구나 쉽게 무료로 접속할 수 있으며, 사용자가 protein input file upload 를 통해 solvation thermodynamic 계산 결과를 도출하여 download 할 수 있다. Solvation free energy 계산은 본 연구실에서 개발한 fluctuation thermodynamics 기술을 사용하여 구현한다. 이 웹사이트를 통해 원하는 단백질의 pdb 파일을 통해 solvation free energy, solvation entropy, solvation energy 를 계산할 수 있으며, decomposition 계산을 통해서는 단백질의 잔기별 residual solvation free energy 를 계산하고 구현할 수 있다. 본 website 에서 solvation thermodynamic 계산은 Linux 의 torque 라는 프로그램을 이용하여 계산을 GPU 서버로 전송시킴으로써 CPU 가 아닌 GPU 에서 수행되도록 만들었다. 본 ProWaVE website 를 통해 단백질의 물 속에서의 거동을 예측하고 구현하며, 나아가 단백질의 소수성, 친수성 부분을 예측하고 이를 통해 단백질의 기능을 이해하고자 하는 많은 연구자들에게 유용한 정보를 제공하고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-433**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Assessment of CCSD(T), MP2, DFT methods for the interactions of peptide backbone and water molecules

강남숙 강영기[1,*]

충남대학교 신약전문대학원 [1]충북대학교 화학과

The CCSD(T), MP2, and dispersion-corrected DFT levels of theory with various basis sets are assessed to understand the interactions of N-methylacetamide (NMA), one of the simplest models for protein backbone, and water molecules. The • B97X-D/6-311++G(d,p) level of theory provided the best results of rotational constants for the structures of NMA and water hexamers consistent with the values from microwave experiments. The • B97X-D/def2-QZVP level of theory provided a good performance for binding energies of NMA and water molecules with RMSD = 0.05 kcal mol-1 with respect to the values at the higher CCSD(T)/CBS-aTQ limit level of theory with aug-cc-pVTZ and aug-cc-pVQZ basis sets. The double-hybrid B2PLYP-D3BJ and meta-hybrid M06-2X functionals with the def2-QZVP basis set resulted the RMSDs of 0.08 and 0.10 kcal mol-1, respectively, with respect to the values at the CCSD(T)/CBS-aTQ limit level of theory, which is similar to the RMSD of 0.09 kcal mol-1 at the CCSD(T)/CBS-TQ limit level of theory with cc-pVTZ and cc-pVQZ basis sets. Thus, the • B97X-D/def2-QZVP//• B97X-D/6-311++G(d,p) level of theory can be a good level of theory to calculate the structures and binding energies of peptide backbone and water molecules around the active sites of protein-ligand complexes.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-434**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Morphology Control of Vertically Aligned Silicon Nanowires with Anisotropic Chemical Etching

홍찬우 정영순 윤일선*

충남대학교 화학과

Here, we studied a simple fabrication of vertically aligned silicon (Si) nanowires with the nanosphere lithography and metal-assisted chemical etching. Self-assembled monolayers of polystyrene (PS) beads were set onto the precleaned Si substrate. The size of the assembled PS beads was subsequently reduced with the oxygen plasma etching (the reactive plasma ion etching). The film of Au with 30 nm thickness was deposited on the substrate using the E-beam evaporator. The PS beads were used as the mask for the Au patterns and the PS beads were detached from the substrate right after the Au deposition. Si nanowires were vertically formed by the catalytic etching of the Si surface under the Au patterned in the mixture solution of HF, H_2O_2, and H_2O (metal assisted chemical etching) and lengths of the Si nanowires were controlled with the reaction time from 0.5 to 3 μm. The morphology of the Si nanowires was controlled with the secondary wet etching. The Si nanowires were anisotropically etched in the mixture etchants of $AgNO_3$ and HF and the etched nanowire were rinsed with a HNO_3 solution sequently. The anisotropic wet etching and rinsing of the Si nanowires were performed repeatedly to change the Si nanostructure from the nanowire to the nanocone.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-435**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Computer Simulations of Intrinsically Disordered Proteins

CHATTERJEE PRATHIT 함시현*

숙명여자대학교 화학과

The investigation of intrinsically disordered proteins (IDPs) is a new frontier in structural and molecular biology that requires a new paradigm to bridge the structural disorder and function. Molecular dynamics simulations and statistical thermodynamics potentially offer ideal tools for atomic-level characterizations and thermodynamic descriptions of this fascinating class of proteins that will complement experimental studies. However, achieving an accurate structural characterization of IDPs via simulations is a challenge because of their sensitivity to inaccuracies in the underlying molecular mechanics force fields. It is also daunting to perform a configuration-space integration over heterogeneous structural ensembles sampled by IDPs to extract, in particular, protein configurational entropy. In this review, we summarize recent efforts devoted to the development of force fields and the critical evaluations of their performance when applied to IDPs. We also survey recent advances in computational methods for protein configurational entropy that aim to provide a thermodynamic link between the structural disorder and protein activity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-436**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Oxygen reduction reaction on the grain boundary between 1T and 2H phase of monolayer MoS2: first-principle calculations for photo-catalytic mechanism process using Real-time time dependent density functional theory

최민 임진오[1,*] 장현주[2,*]

UNIST 화학과 [1]한국화학연구원 화학시뮬레이션센터 [2]한국화학연구원 화학소재연구단

Monolayer MoS2, a two-dimensional transition metal dichalcogenide (TMD) structure material, has been intensively investigated, because of its photovoltaic and photo-catalytic features. It is well-known that monolayer MoS2 has two different phases, 2H and 1T. The 2H phase of MoS2 is a semiconductor with direct band gap about 2.4 eV, and 1T phase of MoS2 has meta-stable metallic phase1. Recently, it was shown that heterostructure containing both 2H and 1T phases can be formed and its microscopic structure is controllable via phase transition2. Such a heterostructure of MoS2 is expected to be utilized in various applications3. We investigated electron dynamics of heterostructure of MoS2, especially focused on the excited electrons from the 2H phase region. The excited electrons transfer to the 1H phase region, and were accumulated in there.This phenomena can be utilized for the oxygen reduction reaction (ORR) catalyst material. For the ORR mechanism, the oxygen molecule should be adsorbed on the catalytic active site easily and the 2 or 4 electrons can be transferred from the active site to the oxygen molecule4. In this study, we have investigated the electron dynamics of the excited-electrons from the 2H phase region and the free energy profile and oxygen adsorption barrier for the ORR catalyst. The electron dynamics was calculated by real-time time dependence density functional theory (rt-TDDFT) developed in our group, and we suggest the new low-dimensional ORR photo-catalyst using the excited-electron in 2H phase MoS2.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-437**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Reversible transformation of hydrophobicity and hydrophilicity of Single-walled Carbon Nanotubes grown on textured Si surfaces

이종택 이준영 양종희 박태훈 이휘건*

한양대학교 화학과

Surface modification of carbon nanotubes (CNTs) has recently attracted a great deal of attention, because the surface characteristics considerably affect applications of CNTs in the fields of biomedical applications, biosensors, catalysts supports, and composites. Wettability of CNTs by liquids is one of the most important surface properties, which normally expressed by contact angle. It is believed that the contact angle of CNTs is determined by chemical composition and surface roughness. Single-walled Carbon Nanotubes (SWNTs) grown on textured Si surfaces by chemical vapor deposition method are Superhydrophobic as the hierarchical structures created by nanostructures on microstructures. The acid oxidation using an acid mixture of nitric and sulfuric acid can readily change the surface of SWNTs grown on textured Si surfaces from superhydrophobic to superhydrophilic. And the reduction by heating in NH3 environment at an elevated temperature can reverse the surface state from superhydrophilic to superhydrophobic. In conclusion, the wettability of SWNTs are controlled by the oxidation and reduction process, significantly facilitate the fabrication and application of composites containing CNTs.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-438**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Diffusion-Influenced Reaction Study on the Compared Efficiency for the Lattice and Brownian Motions

황준필 김태준 김효준*

동아대학교 화학과

Many study of diffusion-influenced reactions use the Monte Carlo simulation, and the simulations have lattice and brownian motions. But, we don't know that which has more efficient. In this prisentation, we study diffusion-influenced reaction by two dynamics systems, and compared efficiency. We proceed that what has the more error, and has the more computer cost in simulation. In this results make the more efficient Monte Carlo dynamics system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-439**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Non-destructive Zinc Oxide Atomic Layer Deposition on Graphene to control electronic properties

박진선 성명모*

한양대학교 화학과

The graphene, a two dimensional material of carbon, has emerged as a highly promising material for next generation electronic devices due to its unique linear band structure, high intrinsic mobility, optical transparency and flexibility. However, for more diverse application of graphene devices, it is essential to control precisely its electrical properties like the Fermi level, carrier concentration, and carrier type while maintaining its excellent properties. So, herein, we suggest a method to tune structural and electronic properties of graphene using atomic layer deposition of inorganic material. By atomic layer deposition of zinc oxide (ZnO) on graphene using a reactive molecular layer, We can deposite uniform, conformal, of good quality with a low density of pinholes of ZnO thin films on graphene. Through π-π stacking between chemically inert graphene and 4-mercaptophenol, conformal deposition of ZnO on graphene was enabled. The electron mobility of graphene TFT significantly enhanced by the n-doping effect without considerably decreasing the hole mobility, compared to the pristine graphene. Also, it has high air stability because ZnO functions as an effective thin-film barrier for graphene devices. This ZnO doping method by atomic layer deposition can be applicable to large scale array of CVD graphene TFT and is well suitable for non-destructive fine-tunable doping of two dimensional materials including not only graphene but also transition metal dichalcogenides (TMDs).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-440**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Conformational Structures of Jet-cooled Substituted N-cyanoindoles and Their Water Clusters: Electronic Spectroscopic and Computational Study

민아름 문철주 안아름 성연국 최명룡*

경상대학교 화학과

N-cyanoindole (n=3 -5) as a derivative of indole has an important intrinsic property for its enormous biological activities in biological systems. We measured the excitation spectra of N-cyanoindole (n=3 - 5) monomer using resonance-enhanced two photon ionization (R2PI) in the gas phase. Then, we obtained UV-UV hole-burning (UV-UV HB) spectra to identify the number of conformers in the N-cyanoindole and their water clusters. We also calculated the ionization and transition energies of N-cyanoindole, (n = 3 – 5) using a various methods (DFT and TD-DFT) with a basis set. The spectroscopic properties of excited states depending on the position of the C≡N group are investigated and discussed by comparing with those obtained from the theoretical calculations.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-441**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Group velocity dispersion measurement for time-zero correction of time-resolved fluorescence spectra

안정수 주태하*

POSTECH 화학과

Fluorescence upconversion is a well-known method to obtain time-resolved fluorescence (TRF) signals or TRF spectra. TRF spectra enables us to capture the excited state dynamics of molecules with less ambiguity than TRF signals. Identifying the exact time-zero position for each detection wavelength prevent the spectra from distortions, when the TRF spectra are scanned in a direct way with high time resolution. Group velocity dispersion (GVD) can play a critical role in the dispersion of time-zero positions for each wavelength component. In this work, we report a direct way to measure the effect of GVD on fluorescence at the fluorescence upconversion apparatus. Measuring the GVD in a direct way allows us to know the dispersion of the time-zero positions of the upconversion apparatus with various modifications. We measured the GVD of a part of the apparatus with a modification in that a cryostat is used as a sample cell, exemplifying the way to utilize the measurement for obtaining the TRF spectra in a modified condition.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-442**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparison of the gas sensing performance of P3HT single crystal nanowire and P3HT thin film ammonia sensor

문서현 성명모*

한양대학교 화학과

In order to comparison of the gas sensing performance of Poly-3-hexylthiophene (P3HT) Thin Film and P3HT single crystal nanowire sensors we fabricated P3HT single crystal nanowire and P3HT thin film ammonia gas sensor using LB-nTM transfer method and spin coating method. The NH3 gas sensor based on single crystal nanowire show responses very low concentration ranging from 0.007 to 25ppm at room temperature and based on thin film sensor responses concentration ranging from 0.008 to 25ppm at room temperature. Single crystal don't have grain boundary and nanowire have a high surface to volume ratio. It is for this reason single crystal nanowrie has been reported high performance rather than thin film. From our measurements we conclude that P3HT single crystal nanowire sensor have high response and detect lower concentration of ammonia gas sensor than P3HT Thin Film sensor.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-443**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Strong optical dipole force exerted on molecules having low rotational temperature

진병권 조범석[1,*]

UNIST 화학과 [1]UNIST 화학과,물리학과

We enhance the optical dipole force acting on molecules by decreasing the molecules’ rotational temperature and aligning the molecular axis with a linearly polarized nonresonant laser beam. The rotational temperature is decreased by increasing a source pressure from 2 to 81 bar. Using the effective polarizability directly pertaining to the optical dipole force, we evaluate the force and the resulting change in the velocity of the molecules. The theoretical calculations are compared with measurements based on the velocity map imaging technique. When the rotational temperature is reduced from 295 to 1 K, the maximum alignment is increased from $<\cos^2\theta> = 0.33$ to 0.92, the average optical force is enhanced by 74%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-444**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

large-scale well-connected graphene grains by selective deposition of inorganic material using atomic layer deposition

NGUYEN VAN LONG 성명모*

한양대학교 화학과

Graphene has drawn enormous attention from both academia and industry because of its excellent transport properties, extremely high mechanical strength, good optical transparency, extraordinary high stability and flexibility. Large-scale CVD-grown preparation of high quality graphene is a requirement for commercial applications in next generation electronics, optoelectronics, and chemical and biosensors. However, large scale CVD-grown polycrystalline graphene containing numerous grain boundaries that would effectively scatter charge carriers, thereby forming highly resistive barriers and adversely affect to decrease of carrier mobility of graphene electronic devices. Here we report, large-scale CVD-grown graphene is enhanced electronic transport properties by selective deposition of hexagonal ZnO on defect-rich reactive and grain boundaries using atomic layer deposition (ALD) technique. Selective deposition of ZnO on CVD graphene is improved notably inter-grain mobility with only a negligible change in the free carrier density. A better connectivity between graphene grains was obtained showing an excellent mobility of graphene TFT. Furthermore, Selective deposition of ZnO on CVD graphene can be successfully applied into wafer-scale arrays on 4-inch Si and polymer substrates, revealing remarkable device-to-device uniformity. In brief, we note that the large-scale well-connected graphene is useful not only for the study of electronic properties of CVD graphene but also for improving other properties of CVD graphene, such as thermal conductivity, mechanical strength, and gas permeability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-445**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

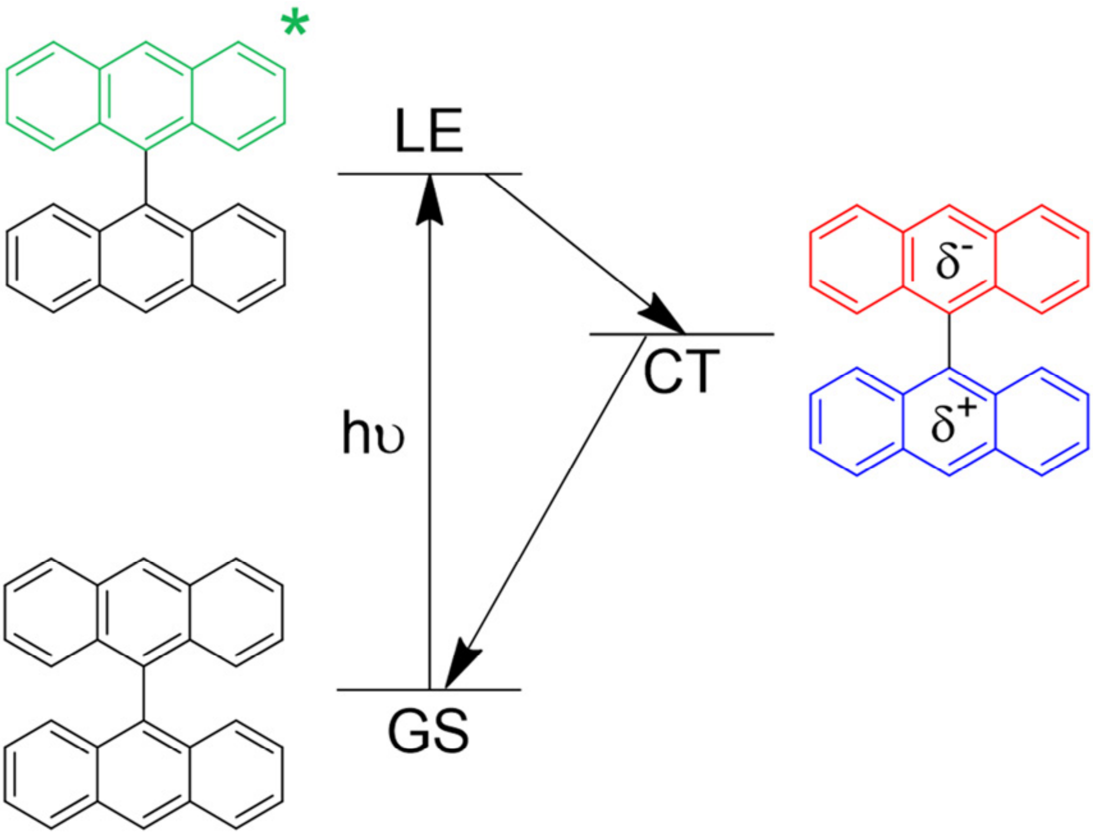
Structural Effects on Symmetry Breaking Photoinduced Charge Transfer of 9,9'-Bianthracene

이창민 주태하*

POSTECH 화학과

Photoinduced symmetry breaking charge transfer (SBCT) is fascinating process because of its importance in biological system and artificial solar energy harvesting system. 9,9'-Bianthracene (BA) is representative model system of the phenomena as it has simple two anthracene moieties (Figure 1). BA undergo SBCT only in polar solvents. Because it has orthogonal torsional geometry in ground state, charge transfer is unexpected process. Thus, not only solvation but structural change is important in SBCT of BA. However, it is still controversial about whether and how structural motion affects overall process. Time-resolved fluorescence with high time resolution (~50 fs) can be a good strategy to obtain clear dynamics as it contains the information of excited state exclusively. Time-resolved fluorescence and its spectrum of BA in non-polar and polar solvents revealed that reaction time in acetonitrile which has fast solvation time may not be same with solvation time (~400 fs). This results can state the importance of structural change on the process.

References
[1] Vauthey, E. Chemphyschem 2012. 13, 2001-2011.
[2] Takaya, T. Hamaguchi, H., Kuroda, H., Iwata, K. Chem. Phys. Lett. 2004. 399, 210-214.


*
LE
CT
hυ
GS
δ⁻
δ⁺

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-446**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of cluster ion secondary ion mass spectrometer

은한준 김정환[1,*] 김남준[*]

충북대학교 화학과 [1]한국기초과학지원연구원 질량분석장비개발팀

SIMS(Secondary ion mass spectrometry) is a technique used to analyze the composition of solid surfaces and thin films by sputtering the surface of the specimen with a focused primary ion beam and collecting and analyzing ejected secondary ions. Especially GCIB (gas cluster ion beam) is less destructive methode than other Primary ion beam source. A new homemade linear TOF(time-if-flight) is being setup in our laboratory. The cluster ion produced Toluene and Argon carrier gas by photoionization. We successfully obtain Huge Toluene$^+$-Ar$_n$ cluster(n≥1000).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-447**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anti-bleaching effect of singlet oxygen scavenger

허 현

한국기초과학지원연구원 광분석장비개발팀

Organic fluorophore is most useful material for contrast agent (fluorescence microscopy, chemo-sensor) and electronic device (DSSC, OLED). Although it has high contrast and high brightness, its intrinsic photo-physics and chemical reaction reduce the lifespan. To speculate fundamental issues, we mainly focus on the unavoidable products, reactive oxygen species (ROS). ROS has high chemical reactivity and are formed as a byproduct of photo-physics or normal metabolism of oxygen. In photo-physics of fluorophore, the spin-flipped molecules in excited state react with ambient oxygen molecules (3Σg) and stochastically generate singlet oxygen (1O2), which is one of ROS. Here, we test the photo-stability of organic fluorophore with optical time-profile under light source and the anti-bleaching efficiency for ROS scavenger. Through visible and near-IR TCSPC, we verify the anti-bleaching effect for singlet oxygen scavengers.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

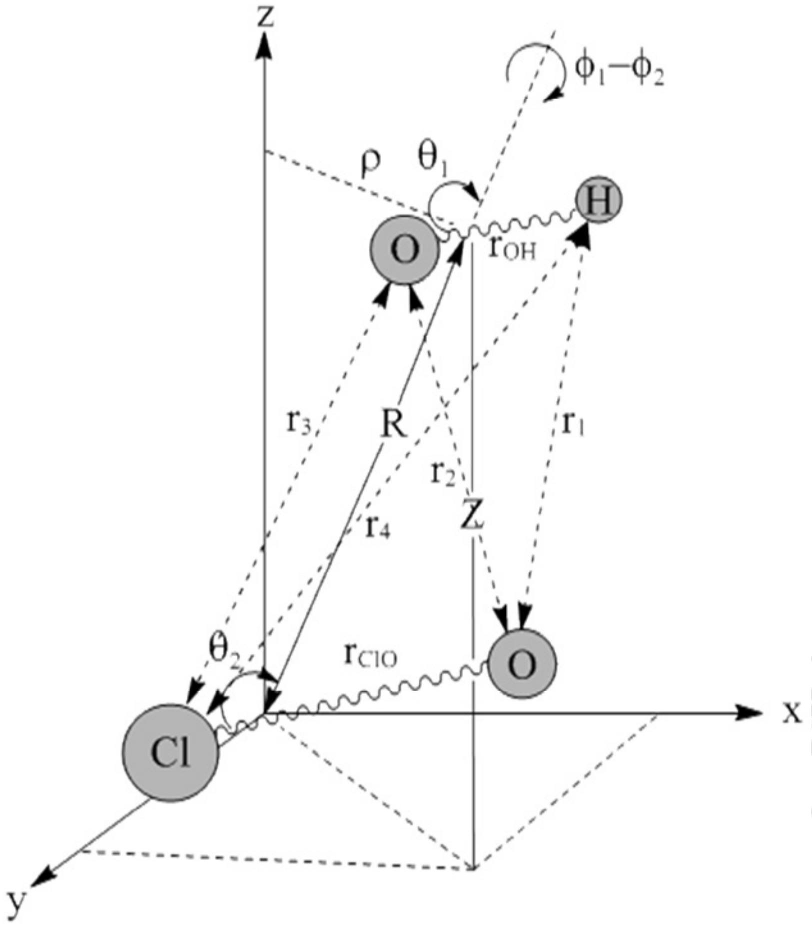
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-448**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Temperature dependence of the reaction of ClO with OH radical

이종백* Hyung Kyu Shin[1] 임소리

전남대학교 화학교육과 [1]University of Nevada, Reno, NV

It has been investigated the temperature dependence of the reaction ClO + OH → Cl + HO_2 using analytic forms of the interaction potential energies in quasi-classical trajectory calculations over the range of room temperature down to 200 K. The overall potential energy is formulated in a form of the London-Eyring-Polanyi-Sato (LEPS) potential terms. Below 300 K, the reaction is attraction-driven and occurs through the formation of a collision-complex ClO ...OH, which is sufficiently long-lived. A negative temperature dependence of the complex mode rate is found between 200 and 400 K consistent with the experimental data reported by various authors. Above 500 K, the reaction occurs primarily through a direct-reaction mechanism. The sum of the complex- and direct-mode rates is shown to describe the reaction over the wide range of 200 - 2000 K.


z
$\phi_1-\phi_2$
ρ
θ_1
H
O
r_{OH}
r_3
R
r_1
r_2
Z
r_4
θ_2
r_{ClO}
O
x
Cl
y

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-449**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Monte Carlo Simulation studies for the efficient methods

김태준 김효준*

동아대학교 화학과

The diffusion-influenced reactions have been tackled with a variety of theoretical approaches and simulation methods. The lattice-based Monte Carlo simulation method is one of the most efficient methods. In this presentation, we show that our adaptive jumping distance methods improve the efficiency of the simulation dramatically. Since the enhanced Monte Carlo simulation methods are especially practical for long time dynamics where many interesting universal laws can be found. We confirmed the efficiency using this methods in the dimension reduction systems, and further the study for the Protein-DNA binding systems to DNA leangh.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **PHYS.P-450**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal enhanced fluorescence of dyes near silver nanosurface

이재범 이대두[1] 송정현[1] 방윤수*

GIST 물리화학부 [1]GIST 화학과

When dye molecules exist close to plasmonic nanoparticles, fluorescence intensities of dye molecules are strongly enhanced by the increase of local electric field or energy transfer between fluorophore and metal nanoparticles and subsequent emission. Excited state dynamics of 4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM) with silver island film (SIF) in methanol showed strong dependence on the excitation wavelength in femtosecond transient absorption measurements. In this work, changes in the excited state kinetics and energy transfers between DCM and SIF in several solvents were studied by femtosecond transient absorption spectroscopy. Although the absorption spectra of DCM are similar in polar and nonpolar solvents, the emission spectra of DCM show large Stokes shift in polar solvents (538 nm in benzene, 562 nm in chloroform, 630 nm in methanol) due to the formation of the intra-molecular charge transfer state. In addition, silver colloidal surfaces with high homogeneity in particles' size and shape were prepared by a kinetically controlled seed-growth method. Excited states dynamics of DCM with the silver colloidal surfaces in composed of nanoparticles in 20-200 nm diameters in several polar and nonpolar solvents will be studied by transient absorption experiments. From these experimental results, detailed mechanisms of MEF and energy transfer between dyes and silver nanosurface will be sought.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **PHYS.P-451**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Improved Energy Conversion Efficiency of Dye-sensitized Solar Cells Fabricated using Open-ended TiO_2 Nanotube Arrays with Scattering Layer

천명환 서정쌍*

서울대학교 화학부

We prepared dye-sensitized solar cells (DSSCs) with enhanced energy conversion efficiency using open-ended TiO_2 nanotube arrays with a TiO_2 scattering layer. As compared to closed-ended TiO_2 nanotube arrays, the energy conversion efficiency of the open-ended TiO_2 nanotube arrays was increased from 5.63% to 5.92%, which is an enhancement of 5.15%. With the TiO_2 scattering layer, the energy conversion efficiency was increased from 5.92% to 6.53%, which is an enhancement of 10.30%. After treating the open-ended TiO_2 nanotube arrays with $TiCl_4$, the energy conversion efficiency was increased from 6.53% to 6.89%, a 5.51% enhancement, which is attributed to improved light harvesting and increased dye adsorption.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-15**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterizing Optical Properties of Palladium-coated Single Gold Nanorods

이소영 하지원*

울산대학교 화학과

Gold nanoparticles have received a lot of interest in the last decade because of their unique optical properties, and their potential applications include catalysis, nanophotonics, and bioimaging. Compared to spherical gold nanoparticles, anisotropic-shaped gold nanorods (AuNR) exhibit two localized surface plasmon resonance (LSPR) modes, longitudinal LSPR mode and transverse LSPR mode. The LSPR modes of AuNRs are strongly dependent on size, shape, and the refractive index of surrounding medium. In recent year, core-shell bimetallic nanorods have also received considerable attention because of their distinct photochemical and photophysical properties. The distinct properties are due to synergetic effect of two different metals. Despite the recent progress in the synthesis of core-shell bimetallic nanorods, our understanding on their optical properties is still very limited at the single particle level. In this respect, we studied optical properties of palladium-coated core-shell AuNRs at the single particle level. The single particle measurement allowed us to eliminate the ensemble error and to gain more specific understanding on their optical properties. In this study, the core-shell nanoparticles were characterized by transmission electron microscopy (TEM), UV-Vis absorption spectrometry, dark-field (DF) microscopy, and differential interference contrast (DIC) microscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-16**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

[발표취소] New Analytical Skills of AFM on the Hair Conditioning Polymer Film

송상훈

LG생활건강 HG.RP

발 표 취 소
본 논문은 발표취소된 논문입니다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL.P-17**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Elucidation of Bortezomib API's morphology in solid state using various analytical methods

고석연 이준희[1] 임병호[2] 김지영[3] 민범찬[1,*]

(주)삼양바이오팜 의약바이오연구소 [1](주)삼양바이오팜 의약바이오연구소 분석센터 [2](주)삼양사 연구소 분석센터 [3](주)삼양사 분석센터

Various analytical methods for the elucidation of Bortezomib API's morphology in the solid state had been developed. The methods applied for different kinds of crystal form include SEM observation, FT-IR structure analysis, DSC thermal transition analysis, XRD crystallography and XPS binding energy study in solid state.Acicular crystal shape of Bortezomib has been observed from SEM, but we assumed that Bortezomib has different crystal pattern which depends on the solvent used for precipitation. Some Bortezomib shows amorphous form but mostly shows perfect crystal form.Moreover we concluded that the Bortezomib should exist as cyclic anhydride of trimeric boroxine form. We used XPS quantitative analysis in solid state and MASS and NMR analysis in solution state for this conclusion.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-18**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Analytical method development for quantitation of residual lactic acid dimer in mPEG-PLA using HILIC column

경규진 이동호[1] 민범찬[1,*]

(주)삼양바이오팜 의약바이오연구소/분석센터 [1](주)삼양바이오팜 의약바이오연구소 분석센터

Lactic acid dimer is one of the process related impurities of mPEG-PLA which can be formed by residual monomer(lactide) ring opening or hydrolytic degradation of mPEG-PLA(methoxypoly(ethylene glycol)-poly(lactide)) copolymer. Hilic(hydrophilic interaction liquid chromatography) is similar to normal-phase LC but uses polar mobile phase such as acetonitrile with a small amount of water. The previous analytical method for quantitation of residual lactic acid dimer in mPEG-PLA was based on C18 column using mobile phase of 95% aqueous solution and it demanded sample to be dissolved in aqueous solution. Because this made residual lactide to be degraded into lactic acid dimer during the preparation of sample solution, it had low stability and could not be reliable and rutine method. Thus, in this work, the quantitative analytical method of residual lactic acid dimer in mPEG-PLA has been developed with hilic column and validated.The chromatographic analysis was performed on Agilent poroshell 120 hilic column(4.6 x 150 mm, 4 μm) using a mobile phase mixture of acetonitrile and 10 mM ammonium acetate buffer(93:7 %v/v) with a flow rate of 1.0 mL/min. The detection was performed at UV wavelength of 210 nm and injection volume was 10 μL. The results of validation showed high specificity and linearity for lactic acid dimer with a correlation coefficient(r) of 1.00 at the concentration range of 1.2~100.0 μg/mL(0.012~1% of test concentration). And the recovery was 100.5%~128.4% and the precision(%RSD) was 0.00~4.32% at 0.05%~1.0% of test concentration. Also, it showed that standard and sample solutions were stable when stored at room temperature for two days.Thus, through this method, we can quantify the residual lactic acid dimer in mPEG-PLA more reliably and efficiently.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-19**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Simultaneous determination of volatile organic compounds (VOCs) with a wide range of polarities in urine by headspace solid-phase microextraction (HS-SPME) coupled to gas chromatography-mass spectrometry

송한나 김종혁 이원용[1] 조성희[*]

한국화학연구원 화학분석센터 [1]연세대학교 화학과

Volatile organic compounds (VOCs), ubiquitous environmental pollutants, are the organic compounds that have a high vapor pressure at room temperature. VOCs have been classified as carcinogen to humans by the International Agency for Research on Cancer (IARC), because they can bind to DNA and cause cell mutations. Therefore, monitoring of VOCs in human urine is very important to evaluate correlation between exposure of VOCs and human disease. We developed the improved analytical method for the simultaneous determination of VOCs with a wide range of polarities in human urine samples by headspace solid-phase microextraction (HS-SPME) coupled to gas chromatography-mass spectrometry (GC-MS). In the improved method, bi-polar carboxen-polydimethylsiloxane (CAR/PDMS) fiber was used for the optimized extraction of 15 VOCs with a wide range of polarities including benzene, toluene, ethylbenzene, xylenes (BTEX), alkylbenzenes, cresols, and naphthalene in human urine samples and the parameters for SPME were optimized. Extracted VOCs from the human urine were effectively separated by GC using mid-polarity column (DB-35, 35% phenylmethylpolysiloxane) and monitored by mass spectrometry using selective ion monitoring (SIM) mode. Under the optimized method, the linearity of calibration curves was higher than 0.993. The limits of detection (LOD) at signal to noise (S/N) ratio of 3 were 0.3-0.6 ng/mL. The coefficients of variation were in the range of 0.1-9.7% for within-day variation and 0.2-14.2% for day-to-day variation, respectively. The present method was highly sensitive and simple for simultaneous determination of VOCs with a wide range of polarities in human urine and could be applied to monitoring and biomedical investigations to check exposure of VOCs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-20**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Determination of bisphenol A in hair samples using liquid chromatography-electrospray tandem mass spectrometry

__이채린__ 김종혁[1] 김성환 조성희[1,*]

경북대학교 화학과 [1]한국화학연구원 화학분석센터

Bisphenol A (BPA), an endocrine disrupter, is widely used to make chemicals for polycarbonate, plastics, beverage containers, epoxy resins, and cash register receipts. BPA is one of the known xenoestrogens, which have weak estrogenic activity and cause obesity, diabetes, breast cancer, and reproductive disorders. Although the levels of metabolomes in hair are relatively lower than those of metabolomes in urine and blood, hair sample has a number of advantages such as easy sampling, long-term storage, long-term history of exposure to the drug and low possibility of sample deformation and contamination. In this study, to investigate extraction and detection of bisphenol A in hair samples, an improved analytical method was developed by liquid chromatography-electrospray tandem mass spectrometry (LC-MS/MS). Hair samples were extracted by an Oasis HLB extraction cartridge after hydrolysis with 1 N HCl and derivatized with dansyl chloride to increase sensitivity. BPA was separated using Shiseido CAPCELL PAK C18 column (2.0 x 100 mm, 3 μm) and a mobile phase consisting of 10 mM ammonium acetate in water and ACN with a gradient program at a flow rate of 0.3 ml/min and was monitored with electrospray tandem mass spectrometry (ESI-MS/MS). The linearity of this method was 0.999. The limits of detection (LOD) at signal to noise (S/N) ratio of 3 was 13 ng/mL. The described method was successfully applied for the extraction and detection of BPA in hair samples and could be used to evaluate and monitor exposure of endocrine disruptor. Also it may play important role to understanding probable endocrine disruptive exposure.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-21**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Determination of Polycyclic Aromatic Hydrocarbons (PAHs) in Human Urine Samples by High-Resolution Gas Chromatography-Mass Spectrometry for Excretion Pattern Study

이선경 김종혁[1] 이상원 조성희[1,*]

고려대학교 화학과 [1]한국화학연구원 화학분석센터

Polycyclic aromatic hydrocarbons (PAHs), the organic compounds formed by at least two condensed aromatic rings, are ubiquitous environmental pollutants that are produced by incomplete combustion of organic materials. PAHs have been classified as carcinogen to humans by the International Agency for Research on Cancer (IARC), because they can bind to DNA, causing mutations. Therefore, the levels of PAHs in human urine samples can be used as an indicator for potential carcinogenesis and cell mutation. In this study, to investigate association between excretion patterns of 18 PAHs in human and carcinogenesis, the analytical method was developed for the measurement of carcinogenic PAHs in human urine using high-resolution gas chromatography-mass spectrometry (HR-GC-TOF/MS). Urine samples were extracted by an Oasis HLB extraction cartridge after enzymatic hydrolysis with β-glucuronidase, arylsulfatase, or β-glucuronidase/arylsulfatase cocktail. The 18 PAHs were separated using Agilent DB-5 MS capillary column (30 m x 0.25 mm, 0.25 μm) and monitored by time of flight (TOF) mass spectrometry with the selected ion-monitoring (SIM) mode. The linearity of this method was over 0.994. The limits of detection at signal to noise (S/N) ratio of 3 were 10 ~ 100 ng/L. The coefficients of variation were in the range of 0.2 -9.0% for within-day variation and 0.4-6.5% for day-to-day variation, respectively. The levels of PAHs in human urine and excretion pattern may play important role to understanding probable carcinogenesis induced by metabolism of PAHs, and the described methods could be used to evaluate and monitor exposure of PAHs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-22**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Single Particle Study on the Optical Property of Pt-coated Core-Shell Gold Nanorods

김근완 하지원*

울산대학교 화학과

Various nanoparticles such as gold nanocubes, gold nanostars and gold nanorods (AuNRs) have been widely studied during past two decades. Recently, bimetallic core-shell nanoparticles have attracted great attention because of their unique optical properties resulted from localized surface plasmon resonance (LSPR) effect. Furthermore, bimetallic core-shell nanoparticles show unanticipated catalytic properties such as high catalytic activity, catalytic selectivity, and better resistance to deactivation. In this study, we investigated individual Pt-coated AuNRs under single particle spectroscopy without ensemble averaging. More specifically, far-field dark-field (DF) microscopy and differential interference contrast (DIC) microscopy were used to obtain optical images of Pt-coated AuNRs and characterize their optical properties at the single particle level.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL.P-23**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Spectroscopic and electrochemical studies of iodine substituted monoclinic $LiFeBO_3$ as a cathode material for Li-ion batteries

이한솔 이영일* 이형동

울산대학교 화학과

There are intensive research activities into alternative electrode materials for the next generation of Li-ion batteries, particularly for use in hybrid electric vehicles and grid scale battery. Monoclinic structured lithium metal borate, $LiMBO_3$ (M = Mn, Fe and Co) for cathode material of Li-ion battery have attracted great interest due to the lowest weight polyanion BO_3^{3-} which offers high theoretical capacity (220mAh/g), environmental friendliness, and high energy density with small volume change of 2%. However, lithium metal borates are considered to have intrinsically low ionic and electronic conductivity which is believed to be the cause of the poor electrochemical performance. Iodine substituted $LiM(BO_3)_{1-x}I_{3x}$ (M=Fe) have been proposed as alternatives to the conventional cathode material. $LiFe(BO_3)_{1-x}I_{3x}$ (x= 0.001, 0.002, 0.003) was synthesized by solid state reaction process. Among them, $LiFe(BO_3)_{1-x}I_{3x}$ (x=0.001) shows the best cycleability. It is characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) and electrochemical test. ^{7}Li MAS NMR was investigated to find lithium local structure of $LiFe(BO_3)_{1-x}I_{3x}$. ^{7}Li MAS NMR spectra of $LiFe(BO_3)_{1-x}I_{3x}$ (x= 0.001, 0.002, 0.003) shows a single isotropic peak with spinning sidebands.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-24**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Customized home-built solid-state NMR probes for biological samples and electronic device

최성섭 정지호 김용애*

한국외국어대학교 화학과

The solid-state NMR has recently developed to investigate insoluble materials. It could be applied to a broad range of organic/inorganic nano-materials including polymers and bio-solids including pharmaceutical drugs and membrane proteins. Solid-state NMR spectroscopy is very valuable to study the structure and dynamics of membrane proteins even though most biological samples on lipid bilayers have high dielectric property due to containing large amounts of lipids, water and salts. We try to make the specific probe with high efficiency and durability for biological samples. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) 1H-15N solid-state NMR probe and a home-built 800 MHz narrow-bore (NB) 1H-15N solid-state NMR probe for these lossy membrane proteins.Li-ion battery and LCD panel have been grown up rapidly as a front-runner in technology-intensive industry. Their microstructural changes are the reason of battery efficiency drop and defective pixel. We will also present a home-built 500 MHz NB 19F-13C solid-state NMR probe with flat-square coil for analyzing LCD panel and 600 MHz NB 19F-7Li solid-state NMR probe with solenoidal coil for investigating Li-ion battery. These were the first application for the in-situ analysis of LCD panel and in-situ analysis of Li ion battery pack samples. These two probes provide high efficiency and good RF homogeneity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-25**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Strategies employed in the characteristics of antimicrobial peptides with enhanced activities derived from Lactophoricin

정지호 김지선 김용애*

한국외국어대학교 화학과

In recent years, spread of antibiotic resistance bacterial pathogens have been considerable interest in investigations of new class of antimicrobial molecules, antimicrobial peptides (AMPs). AMPs are usually relatively short positively charged polypeptides and exhibiting amphipathic character. Despite significant differences in their structures, all AMPs discovered share the ability to interact with cellular membranes, thereby disrupting membrane organization. Lactophoricin (LPcin), a cationic amphipathic peptide consists of 23-mer peptide, was currently utilized as the framework to design the novel analogs and study the effect of peptide hydrophobicity/hydrophilicity, amphipathicity on antimicrobial activities. LPcin analogs were designed and modified to enhance antibacterial activity using conservative sequence change. Three promising candidates were selected among LPcin analogs using bacterial killing and growth inhibition assays against Gram-negative and Gram-positive bacteria. We successfully overexpressed LPcin analogs in the form of fusion protein in Escherichia coli and purified them from the cell extracts with many biophysical techniques. In order to elucidate the structure-antibiotic activity relationships of the peptides, we studied the correlation between the modified conformation of LPcin analogs and their antimicrobial activity using various spectroscopic methods like MALDI-TOF MS and CD spectrometry, as well as 1D/2D solution NMR spectroscopy and 1D/2D solid-state NMR spectroscopy in membrane mimic environments. The structural calculations of LPcin analogs using Discovery Studio 2016 were also used to refine the orientational information of 3D structure and topology based on 2D SAMPI4 solid-state NMR spectra.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-26**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study of the electrochemical performance for nickel substituted olivine-monoclinic complexes as a cathode material for Li-ion batteries

이지원 이영일* 박재영 지민수

울산대학교 화학과

The olivine structured LiMPO$_4$ (M= Fe, Co, Ni) as an attractive cathode material for Li-ion batteries has been investigated due to low cost, eco-friendly, and structural stability. However, olivine materials have relatively poor electrochemical performance compared to other structure of cathode materials such as layered structure $LiCoO_2$, spinel structure $LiMn_2O_4$, and monoclinic structure $LiFeBO_3$. It is known that the mixing of olivine and monoclinic structured material is improved the specific capacity. Moreover, nickel substitution in metal site is suggested in this presentation to increase operate voltage and conductivity. The olivine-monoclinic complex materials have been synthesized by solid-state reaction using planetary mill. The morphology, compositions, and electrochemical performance of the synthesized sample were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), cycling test, galvanostatic charge-discharge measurement, etc.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-27**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Quantitation of arsenic species in white rice and brown rice using LC-ICP-MS System

박미선 김관수*

동일시마즈(주) 지원본부

Rice is one of the agricultural products including a relatively significant amount of arsenic in which the ratio of inorganic arsenic is commonly known to be high. Codex Alimentarius Commission held in July 2014 decided to be 0.2 mg/kg over the maximum content of inorganic arsenic in polished rice. Arsenic species have each inherent poisonous property. The poisonous property of inorganic arsenic is known to be higher than that of organic arsenic. An LC-ICP-MS system which connects an inductively coupled plasma mass spectrometer (ICP-MS) in-line with a high-performance liquid chromatography (HPLC) system allows the high sensitive and high accuracy measurement of arsenic species. The quantitation of inorganic arsenic species [As(III) and As(V)] and dimethylarsinic acid in white rice and brown rice was accomplished by connecting the ICPMS-2030 in-line with a HPLC system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-28**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

피톤치드가 첨가된 PSA의 성능평가에 관한연구

김경석 전보현 서예지 김성호*

순천향대학교 화학과

피톤치드는 식물에 존재하는 향으로써 스트레스 완화작용, 항균작용 등이 알려져 있으며, 방향제, 천연 세제 등 여러 형태로 이용되고 있다. 본 연구에서 점착제 층에 피톤치드를 첨가하여, 패치를 제작하고, 피톤치드의 유효성능유지기간, 점착력, 유지력등을 측정하는 방법으로 그 성능을 평가하였다. GC-MS 를 이용한 정성분석, HPLC 를 이용하여 정량분석을 실시하였으며, Ball Tack, peel strength, 유지력등을 측정하여, 성능이 우수한 피톤치드 패치를 개발하였다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-29**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

라벤더 향이 첨가된 패치의 점착성능 평가

전진 유하나 문지연 김성호*

순천향대학교 화학과

최근 천연오일의 효능이 밝혀짐에 따라 다양한 형태의 향 이용 방법이 개발되고 있다.그 중 수명과 효능을 오래 지속시키는 방법의 하나로 패치가 이용되고 있다. 패치 제작시 PSA 에 라벤더 오일을 첨가한다. 본 연구는 패치의 PSA 에 첨가된 라벤더오일을 GC-MS 와 HPLC 를 이용하여 정성, 정량 분석하여 첨가된 라벤다의 유효 시간을 측정 하였으며, 향의 함량변화에 대한 초기점착력, 유지력 변화등을 측정하는 방법의 패치의 성능을 평가 하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-30**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enantioseparation of acidic chiral compounds on a clarithromycin-zirconia hybrid monolith by capillary electrochromatography

김미연 박정학*

영남대학교 화학과

A weak anion exchanger chiral selector, clarithromycin-incorporated zirconia hybrid monolithic (CLA-ZHM) capillary column was prepared by sol-gel technology. A sol solution consisting of 5.5 mM of polyethylene glycol, 1 mM of water, 3 mM of acetic acid, 2 mM of formamide, and 0.04/0.96 ratio of CLA-TEOSPC/Zr-Bu resulted in a homogeneous monolith having well defined through-pores and tightly anchored to the capillary wall. The CLA-ZHM column was employed for capillary electrochromatographic enantioseparation of ten acidic chiral drugs in mobile phases consisting of acetonitrile (ACN), methanol (MeOH) and triethylamine (TEA)-acetic acid (AcOH) buffer. Effects of ACN/MeOH ratio, AcOH/TEA ratio and their concentrations, and applied voltage on chiral separation were investigated. Baseline resolutions of all the compounds were achieved with a mobile phase of 70:30 (v/v) ACN/MeOH containing 255 mM AcOH and 17.4 mM TEA under the applied voltage of –10 kV at 25 ^{o}C.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-31**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Hyperpolarized Silicon Nanoparticles as Biocompatible Contrast Agents for 29Si Magnetic Resonance Imaging

서형림 최익장 고혜지 공경헌 박희정[1] 정회일[2] 이영복[*]

한양대학교 응용화학과 [1]한국기초과학지원연구원 서울서부센터 [2]한양대학교 화학과

Silicon-based nanoparticles have been attracting a lot of interest in the field of biomedical applications due to their biocompatibility and biodegradability in vivo, as well as their flexible surface chemistry. Here, we demonstrate two different synthetic approaches in order to yield various nano-sized silicon nanoparticles (Si NPs) ranging from 5 nm to 500 nm as hyperpolarized contrast agents for magnetic resonance imaging (MRI). i) The particles were synthesized by means of a chemical reduction of micelles formed by mixing silicon tetrachloride and alkyltrichlorosilane. ii) Magnesiothermic reduction of silica was also processed to produce Si NPs. The Si NPs have many great benefits to the hyperpolarized MR imaging. Since a core region of the crystalline Si NPs is mostly protected from a main relaxation source, such as paramagnetic centers existing at surface defect sites, the Si NPs show extremely long depolarization times (usually longer than 30 mins), resulting in high MR image contrast with minimum or no background signals. In addition, paramagnetic centers on the surface defect sites play a pivotal role in generating MR signal enhancement induced by dynamic nuclear polarization (DNP) mechanism, thereby not necessary to add external radical sources. In conclusion, these features and benefits convincingly suggest that the Si NPs can potentially be used as a biocompatible, targetable, and hyperpolarized MRI contrast agents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-32**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and characterization of Silicon/reduced Graphene oxide composite film as anode for lithium ion batteries

이상훈 김용재 손빛나 최진영 이호춘[1] 이창섭[*]

계명대학교 화학과 [1]DGIST 에너지시스템공학

Silicon (Si) has been used as one of the most attractive anode materials for lithium-ion batteries because of its large theoretical capacity, high safety, low cost and environmental benignity. However, Silicon-based anode material needs to overcome the structural change of the solid-electrolyte interphase due to the large volume change during cycling. To resolve these problems, we have synthesized Si/rGO composite using graphene with superior conductivity, large specific surface area and flexibility. The Graphene oxide(GO) solution was deposited on the copper foil for 10 min to form a GO layer. Then the Si-containing solution was deposited for 5 min to form a Si-doped layer. Finally, the multi-layered structure was obtained by depositing GO and Si-doped layers alternately. After heat treatment by thermal chemical vapor deposition(CVD), the resulted Si/rGO composite film on copper foil was obtained. The characteristics of Si/rGO composite were analyzed by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of Si/rGO as anodes of Li ion batteries were investigated using coin cell and battery tester.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-33**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Electrochemical Performance of Transition metal-coated Carbon Nanofibers as Anode Materials for Lithium Secondary Batteries

최진영 현유라 황은정 박희구[1] 이창섭*

계명대학교 화학과 [1]계명대학교 화학시스템공학과

In this study, transition metal coated carbon nanofibers (CNFs) were synthesized and applied as anode materials of Li secondary batteries. The CNFs/Ni foam was put into the 0.01 M transition metal solutions after the CNFs were grown on Ni foam via chemical vapor deposition (CVD) method. The transition metal coated CNFs/Ni foam was dried in a dryer at 80 ℃. The morphologies, compositions, and crystal quality of transition metals/CNFs/Ni foam were characterized by SEM, EDS, XRD, and Raman spectroscopy. The electrochemical characteristics of transition metals/CNFs/Ni foam as anode of Li secondary batteries were investigated using three-electrode cell. The transition metals/ CNFs/Ni foam was directly employed as a working electrode without any binder, and lithium foil was used as the counter and reference electrodes. 1 M $LiClO_4$ was employed as electrolyte and dissolved in a mixture of propylene carbonate (PC) : ethylene carbonate (EC) in a 1:1 volume ratio. The galvanostatic charge/discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. In particular, synthesized transition metals/CNFs/Ni foam showed the highest retention rate (41%). The initial capacity (670 mAh/g) was reduced to 275 mAh/g after 30 cycles.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

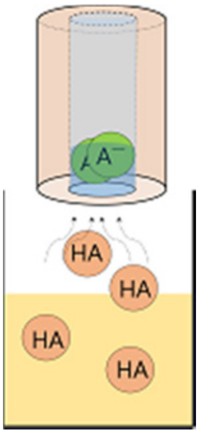
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-34**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Headspace intube microextraction for capillary electrophoresis mass spectrometry for analysis of hydrophilic volatile molecules

권준엽 최윤정 정두수*

서울대학교 화학부

Capillary electrophoresis mass spectrometry (CE/MS) is appropriate analysis method for small amount of samples. However CE/MS lacks of online sample extraction method. We previously made headspace single drop microextraction (HS-SDME) for CE/MS. HS-SDME showed high enrichment factor (EF) and reproducibility. But HS-SDME required improvised outlet vial for drop formation which needs skillful handworks and risks electrospray needle conditions. Headspace intube microextraction (HS-ITME) uses no drops, only exposed area of acceptor in capillary section. HS-ITME shows lower EF than HS-SDME, but HS-ITME requires no improvised vial or modification to electrospray ionization area. We applied short chain fatty/organic acids and chlorophenols as examples. EF, comparing with normal CE/MS, showed 20~30 for 15 min extraction under room temperature. The HS-ITME is expected to increase effectiveness of CE/MS.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-35**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Application of Ultra-high resolution 2-Omega FT-ICR MS for the Analysis of Complex Mixture

조은지 김성환*

경북대학교 화학과

It is important to understand the chemical compositions of complex mixture including crude oil. There are many studies on analyzing the chemical compositions of crude oil using ultrahigh-resolution mass spectrometry (UHR-MS). Analysis of crude oil using Fourier transform ion cyclotron mass spectrometry (FT-ICR MS) has a great advantage. In those application, resolution and mass accuracy plays a key role in accessing accurate chemical compositions. The resolution of FT-ICR MS is increased proportional to the measured frequency. A new technique called “2-Omega” has been recently developed. In the technique, two pairs of electrodes comprising FT-ICR MS detector cell are used for detection. Therefore, the measured resolution is supposed to be doubled compared to the old design where only one pair of electrodes is used for detection. In this study, ultrahigh resolution mass spectra of crude oil were obtained and presented. The obtained mass accuracy and resolution are presented. The resolution of 2-Omega FT-ICR MS spectra were well over one million. The data were also examined to check the existence of 1-Omega peaks because they can cause mis-interpretation. The data presented in this study clearly shows that 2-Omega FT-ICR MS can be very useful in the analysis of complex mixture such as crude oil. To the best of our knowledge, this is the first report on the application of 2-Omega FT-ICR MS to study crude oils.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-36**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Energy Dependent Tandem Mass Spectrometry Analysis for Structural Identification of Polycyclic Aromatic Hydrocarbons

하지현 김성환*

경북대학교 화학과

PAH (Polycyclic Aromatic Hydrocarbon) compound are common molecules found in the environment as well as Crude Oil. Some PAH are significant pollution source in the human body or the environment. In addition, PAHs include several isomers. It is important to analyze PAH compounds including structural isomers. One of the most widely used methods for PAH compounds is Liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). However, only a few publications reporting high resolution MS/MS spectra of PAHs are currently available. In addition, further limited number of publication is available focused on energy dependent MS/MS spectra of PAHs. In this study, it is hypothesized that obtaining MS/MS spectra with different collision energies and comparing the energy dependent pattern can be a useful tool to distinguish PAH isomers. To test the hypothesis, MS/MS spectra of 50 PAH compounds were obtained at various collisional energy and fragmentation patterns of PAHs depending on collisional energy were compared. Our results show that PAH isomers could be successfully distinguished from their significantly different relative ion intensity in the spectra obtained with various collision energies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-37**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

In situ Monitoring of Thermal Crosslinking Reaction and Residual Vinyl Group of Re-adhesive Organosilicon by VT-NMR

설혜원 이태희[1] 이태곤[1] 김정권* 김종혁[1,*]

충남대학교 화학과 [1]한국화학연구원 화학분석센터

The re-adhesive property of organosilicon is dependent on the residual vinyl group after the crosslinking reaction of hydrosilylation between vinyl group(Si-V, main chain) and hydrosilyl group(Si-H, crosslinker). When the vinyl group remains, we cannot expect good re-adhesive property because of adhesion over time. In this study, the end-point of crosslinking reactions was determined by variable temperature nuclear magnetic resonance(VT-NMR) spectroscopy. The relationship between adhesion and the residual vinyl group was confirmed by monitoring the crosslinking reaction. Our experiments were done with organosilicon mixture of main chain and crosslinker which has the end- or side-chain vinyl group and hydrosilyl group. Temperature was raised from 298 K to 373 K at a rate of 1.25 K/min and the spectra were recorded for a minute at each 5 K. The end-points of crosslinking reaction were determined by the loss of vinyl group signals and the appearance of crosslinking network($Si-CH_2-CH_2-Si$) signal in distortionless enhanced by polarization transfer(DEPT) spectrum. In case of the most vinyl-terminated poly-dimethylsiloxane, vinyl group signal was disappeared below 373 K. When a vinyl group is positioned beside backbone(vinyl-methylsiloxane), however, it still remained until 373 K. Additionally, we also investigated samples from a supplier and compared the results with our initial work. The adhesive remnant indexes(ARI) were almost the same when the vinyl group signal disappeared, while it changed when the vinyl group signal remained.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-38**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization of the Weathered Oil and Soil Extract Originated from Crude Oil Spill Site by Paper Spray Ionization Mass Spectrometry

김동휘 차상원[1] 김성환*

경북대학교 화학과 [1]한국외국어대학교 화학과

Oil spills have drawn the attentions of the researchers for their potential threats as well as direct influences to the environment and human beings.Once oil is spilled that goes through various reactions such as biodegradation and photodegradation, so that chemical compositions of the spilled oil are changed by weathering process. Besides, those reactions produce various toxic materials.Petroleomics using ultra-high resolution mass spectrometer(UHR-MS) has emerged as a powerful technique for analyzing petroleum and its product. ESI, APPI, and APCI are the most common ionization techniques for characterization of petroleum products. Even though those are very useful techniques, there are some limitations associated with solvent selection, sample amount and clogging problem. Therefore, application of new ionization technique can be beneficial.Recently developed paper spray ionization (PSI) is fast and convenient ionization method for the direct analysis of complex mixtures with minimum sample preparation. In addition, ionization and subsequent MS analysis can be done with small amount of sample when compared with aforementioned ionization techniques.In this study, weathered oil and soil extract from Hebei Spirit oil spill site in Taean have been characterized by paper spray ionization mass spectrometry.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-39**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Investigating Photo-oxygenation tendency of Compounds with OLED Basic Structures by PSI Orbitrap and MALDI-TOF MS and Theoretical Calculation

박은영* 하지현 김성환

경북대학교 화학과

Organic light editting diode (OLED) utilize organic compounds that emit light after receiving electrical signals through electrical currents. The OLED is often commercially used to make displays for computers, smart-phones and various other electronic devices. However, when the components of OLED are photo-oxidized, impurities are created and the color of the display is changed. Compounds used for OLED typically have anthracene as basic structure. There are many compounds substituted at 9, 10 positions of anthracene. However, the effect of side chain on the oxidation rate has not been investigated yet. Therefore, in this study, samples having anthracene as core structure and 9 and/or 10 positions substituted with phenyl, methyl, or naphthyl groups were studied. The samples were oxidized with UV lamp under flow of oxygen gas. The observed rate of oxidation was different for each functional group. The Paper Spray Ionization (PSI) and Laser Desorption Ionization (LDI) mass spectrometry were used to analyze the oxidized samples. Theoretical calculations have been performed to explain the observed data.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-40**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study on Molecular Dynamics (MD) Simulations for Long Alkyl Chain Aromatic Compounds by using Ion Mobility Mass Spectrometry

임동완 김성환*

경북대학교 화학과

Travelling Wave Ion Mobility Spectrometry Mass-Mass Spectrometry (TWIMS-MS) is technique used to study shape and conformation of small molecules and proteins in gaseous ions. Furthermore, the analysis for Polycyclic Aromatic Hydrocarbons (PAHs) compounds in Crude oil is still one of important modern research issues. Especially, a detailed structural characterization of the involved PAHs compounds with alkyl chains is one of the remaining challenges in petroleomics. Our previous study (Ahmed, A. et al., Anal.Chem. 86, 3300-3306, 2014) has already shown the advantage of combining two well established MS techniques with theoretical Collisional Cross Section (tCCS) calculations to increase the amount of information gained as well as to determine the molecular structures of aromatic compounds. However, the result of previous study was limited to determine non-alkylated or short alkyl chains aromatic compounds. In this study, we employed temperature dependent molecular dynamic (MD) simulation to improve the CCS calculation accuracy, especially for long alkyl chain containing aromatic compounds. The Molecular Dynamic Simulation results of all the compounds correlates better with experimental results at high temperatures.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-41**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Non-invasive detection of inner layer materials in turbid media using Deep Raman Spectroscopy

조영호 지민호 배창현 박찬량[1,*] 김형민*

국민대학교 생명나노화학과 [1]국민대학교 화학과

One of the most goals of the analytical technique in industrial fields is the provision of chemically fingerprinting, non-invasive method for monitoring the raw material composition in opacity media such as poly-ethylene case. Recently, the deep-Raman techniques play an important role in non-invasive and chemically specific analysis methods such as spatially-offset Raman spectroscopy (SORS). In this study, we demonstrate deep layer materials in turbid media without unpackaged using non-invasive deep Raman technique such as spatially offset Raman spectroscopy (SORS), line illumination spatially offset Raman spectroscopy (L-SORS) and line illumination one shot imaging techniques. Furthermore, the deep Raman methods are adopted to confirm their possibility for raw materials monitoring without unpackaged in pharmaceutical and industrial fields.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-42**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Non-destructive Analysis of Traditional Korean Pigment Using Resonance Raman Scattering

송시원 박수빈 유익한 김규호[1,*] 박찬량[2,*] 김형민[*]

국민대학교 생명나노화학과 [1]공주대학교 문화재보존과학과 [2]국민대학교 화학과

Raman spectroscopy is the powerful spectroscopic tool that non-destructive in investigation of chemical compounds of materials. The Raman spectroscopy as a non-destructive methodology is demonstrated of published literatures [1]. It has not only non-destructive analysis but also a variety of advantages. It measures molecular vibration mode from scattering light according to lasers. Therefore it detects to the chemical composition, bonding, and structure of the sample material [2]. Furthermore, the Raman spectroscopy has benefit such as in situ monitoring and portability. These characteristics provide sensitive measurement to analysis at art and cultural properties because of the Raman spectroscopy do not damage at sample that have substantially historic worth and also provide a chemically fingerprint about the identification of materials. However, pigments had variable colors interrupt to measure Raman signal because of its radiating fluorescence. Therefore, we study identification of traditional Korean pigments using variable lasers. These are important to avoid fluorescence and take enhanced Raman signal from the resonance Raman scattering (RSR) effect that increases scattering efficiency because of that is related region of electronic state [3]. Resonance Raman measurement was performed a microscope (Olympus Bx73) that coupled to a spectrometer (Andor Shamrock 303i) with charge coupled devices (Andor iDus 420) using by 488 nm Ar-ion, 532 nm diode, and 632.8 nm He-Ne lasers. The pigment is used lumber painted Korean traditional pigment such as painted Sungnyemun Gate. In conclusion, we study using the resonance Raman methodology for analysis of pigments that have color be of help chemical identification and make database. It be of help for preservation and restoration Korean cultural properties.1.G. Burrafato, M. Calabrese, A. Cosentino, A. M. Gueli, S. O. Troja, and A. Zuccarello, ColoRaman project:Raman and fluorescence spectroscopy of oil, tempera and fresco paint pigment, Journal of Raman Spectroscopy 35, 879-886 (2004).2.G. D. Smith, and R. J. H. Clark, Raman microscopy in archaeological

science, Journal of Archaeological Science 31, 1137-1160 (2004).3.D. Gill, R. G. Kilponen, and L. Rimai, Resonance Raman Scattering of Laser Radiation by Vibrational Modes of Carotenoid Pigment Molecules in Intact Plant Tissues, Nature 227, 743-744 (1970).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-43**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Carbomylated azithromycin-incorporated zirconia hybrid monolith for enantioseparation of acidic drugs using non-aqueous capillary electrochromatography

dixitshuchi 박정학*

영남대학교 화학과

Carbomylated derivatives of two antibiotics, namely, clindamycin phosphate (CLIP) and erythromycin (ERY) were successfully employed as co-precursors, in combination of zirconium tetrabutoxide as a precursor, to prepare chiral organic-zirconia hybrid monoliths (i.e., CLIP-ZHMs and ERY-ZHMs, respectively) via a single-step in-situ sol-gel approach in our previous works [1,2]. Their superiority over chiral organic-zirconia/silica monoliths, prepared by post-modification approach, in terms of better enantioresolution and enhanced stability inspired us to prepare ZHMs based on an another antibiotic, azithromycin (i.e., AZI-ZHMs). Monolithic columns were employed for capillary electrochromatographic enantioseparation of acidic chiral drugs in mobile phases consisting of acetonitrile (ACN) and methanol (MeOH) as organic modifiers and, acetic acid (AcOH) and triethylamine (TEA) as electrolytes. The effects of composition of mobile phase and applied voltage on chiral separation were investigated by using ketoprofen as a representative analyte. Baseline resolutions (i.e., Rs >1.5) were obtained for six acidic drugs (namely, ketoprofen, suprofen, carprofen, flurbriprofen, ibuprofen and warfarin) using a mobile phase consisting of 70/30 (v/v) ACN/MeOH with 240 mM AcOH and 20 mM TEA. The relative standard deviations for resolution values regarding column to column and batch to batch repeatability were less than 2.5% (for n=3) under optimized conditions indicating satisfactory stability of columns and reproducibility of column preparation process. [1]Dixit, S., Park, J. H., J. Chromatogr. A 2015, 1416, 129-136.[2]Tran, L. N., Dixit, S., Park, J. H., J. Chromatogr. A 2014, 1356, 289-293.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-44**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Laser Desorption/Ionization Mass Spectrometry Analysis of Boron Nitride

배광태 조수경[1,*] 유해욱[2]

국방과학연구소 4본부 2부 [1]국방과학연구소 4본부-2부 [2]국방과학연구소 4본부2부

Laser desorption/ionization (LDI) mass spectrometry is one of useful analytical instruments in identifying high energy species from various precursors. We have been investigating nitrogen-rich high energy species starting from azoles, azides, and other compounds generating nitrogen-rich species [1]. Boron nitride is one of promising precurors which may generate highly energetic nitrogen-rich species. In addition, boron species are also known to hive high energies. We performed LDI experiments on solid boron nitride and analyzed with time-of-flight mass spectrometry (TOF MS). Various ionic BxNx clusters of B+, B2+, BN+, N2+, B3+, B2N+, N4+, B3N2+, B4N3+ were identified in positive MS mode. Further, we will present energy diagrams and reaction mechanisms of these highly energetic species.[1] Cho, S.G.; Bae, K.T.; Goh, E.M. Bae, S.W.; Shin, I.-S. Bull Korean Chem. Soc, 2016, 37, 99-102.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-45**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Relative Quantitation of N-linked Glycans in Rice using Metabolic Isotope Labeling by Mass Spectrometry

서현경 김진화 임재민*

창원대학교 화학과

Glycosylation is one of the most common post-translational modifications in biological system. Glycan play significant roles for a wide range of biological processes regulating such as cell-cell interactions, cell division and adhesion, cellular recognition, immune response, and protein stability. For the purpose of understanding the biological relevance of glycans, many mass spectrometry based methods have been developed for the relative quantitation of glycan.Herein, we describe a new *in vivo* labeling method either normal or heavy glucose to tag glycans from rice culture. Isotopic glucose enters the glucose metabolic pathway, which in turn produces nucleotide sugars precursors that are subsequently used for all glycan biosynthesis.Thus, each of sugars in glycan occur a mass shift as much as 1 Da. For glycan containing five sugars, occurs a mass shift of as much as 5 Da. A method for relative quantitation of glycans by ratio of normal glucose labeled glycan and heavy glucose labeled glycan.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-46**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Simultaneous Determination of Estrogens in Environmental Aqueous Samples by Dispersive Liquid–Liquid Microextraction and HPLC/UV-Vis

문연주 조현우[1] 명승운*

경기대학교 화학과 [1]경기대학교 자연과학화학과

The objective of this study was to optimize dispersive liquid–liquid microextraction (DLLME) parameters for the simultaneous sample preparation of five steroidal estrogens (estrone (E1), 17α-estradiol (αE2), 17β-estradiol (E2), 17 α-ethinylestradiol (EE2), and estriol (E3)) from environmental aqueous samples. Estrogens were extracted and concentrated simultaneously an aqueous sample using dispersive and extraction solvents, and chromatographic separation and quantitative analysis were performed by an HPLC/UV-Vis system. It was evaluated optimum parameters for the effects of the combination of dispersion and extraction solvent, ionic strength, and sample pH. The optimized results gave increased enrichment factors (EF = 28.4–69.4). From the established extraction condition, the limits of detection and quantification in the spiked samples were in the concentration ranges 0.03–0.07 mg/L and 0.10–0.23 mg/L, respectively. The method gave good linear calibration curves with correlation coefficients (r_2) of 0.9990–0.9995 in the 0.10-8.00 mg/L. The relative recoveries and standard deviation in the calibration ranges were 99.1–116.6% and 0.6–4.2% (RSD), respectively. The proposed method, which is fast, simple, inexpensive, and environmental friendly, can be applied to the effective and simultaneous analysis of five steroidal estrogens from environmental aquatic samples.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-47**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Using EME for Determination of NSAIDs by HPLC-UV

김진문 조현우[1] 명승운[*]

경기대학교 화학과 [1]경기대학교 자연과학화학과

The electromembrane extraction(EME) is one of the liquid phase microextraction(LPME) which can extract and concentrate the analyte from aqueous matrices such as urine and plasma effectively. This method was applied to analysis of six Non-steroidal anti-inflammatory drugs(NSAIDs) in aqueous samples. The parameters such as pH of acceptor and sample, stirring speed, voltage, support liquid membrane(SLM), and extraction time were optimized. Simultaneous chromatographic separation of six NSAIDs by HPLC-UV/Vis system was achieved on an Eclipse XDB-C18 (4.6 mm i.d. × 150 mm length, 5 ㎛ particle size) column using gradient elution with 0.1 % formic acid and methanol. 0.1 % formic acid and methanol start to 20:80 and after 7minutes, compositon and flow rate are changed to 15:85, finally, back to the first condition after 5minutes. After the extraction, 5 ㎕ of extract was directly injected into the HPLC-UV system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-48**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

FT-IR microscopic study of human hairs in various pH solution

김혜영 권오선 유수련[1] 신관우[2,*]

서강대학교 화학과 [1]서강대학교 화학과,바이오계면연구소 [2]서강대학교 화학과 및 바이오융합과정

In this research, natural and intact hair is used and experiments are performed within pH range from 1 to 12. Given that nitrogen oxide is the major cause of acid rain, nitric acid was used for making acidic solution and for the basic one, normal potassium hydroxide was used. In each pH, cross-section images and IR spectrums are obtained with FT-IR microspectroscopy. Since a hair fiber can be divided into outer layer(cuticle) and inner part(cortex), comparisons between these two parts are also made in each section. From the controlled experiments, we will present how the human hairs can be affected and the detailed analysis of each protein component in various pH condition will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-49**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Headspace in-tube microextraction of dichlorophenols using a commercial capillary electrophoresis instrument

최윤정 정두수*

서울대학교 화학부

Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are commonly employed for headspace (HS) extraction, which is useful for the concentration of volatile materials in a complex matrix. Among LPME methods, single drop microextraction (SDME) is widely used for HS extraction to be off-line coupled with GC and LC. By forming a single acceptor drop at the tip of a capillary using a commercial capillary electrophoresis (CE) instrument, we showed that SDME can be easily in-lined coupled with CE to achieve high sample enrichments in a short time. However, it is difficult to hang a drop of very small volume to a separation capillary in the HS stably for long extraction. Recently this problem was solved by in-tube microextraction (ITME) using the liquid plug inside the capillary as an acceptor phase without hanging a drop. HS-ITME-CE was performed to enrich dichlorophenol in an aqueous solution. To promote the evaporation of the acidic dichlorophenols into the HS as neutral forms, the donor was acidified by adding HCl. To promote back extraction from the HS, a short acceptor plug of 400 mM borate buffer of pH 9.3 was used. The subsequent CE was carried out using a run buffer of 240 mM borate buffer of pH 9.2. With a 15-min extraction at 80°C, dichlorophenols were enriched about 300 times.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-50**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Automated liquid extraction surface analysis in-line coupled with sweeping for rapid and direct analysis of a solid surface sample

이호균 최윤정 정두수*

서울대학교 화학부

High performance separation and many other advantages such as a small volume sample requirement of capillary electrophoresis (CE) come from the fact of using a narrow-bore fused silica as a separation column. However, the small dimension of the detection path length causes poor detection sensitivity. To overcome this, sample preconcentration technique is needed. There were many preconcentration methods coupled with CE, but almost used liquid sample or homogenized solid bulk sample. Liquid extraction surface analysis (LESA) is a direct surface-sampling technique avoiding the dilution from sample pretreatment procedures including homogenization of a bulk sample. LESA was in-line coupled with homemade CE-laser induced fluorescence (LIF), but homemade CE was operated manually and sample was injected by gravity, so whole extraction procedure needed ~20 minutes. In this study, commercial CE instrument was used for rapid and automatic LESA, and extraction only took ~2 minutes. For separation neutral pesticides efficiently, we use sweeping for detect choloorantranili, kresoxim-methyl and paraclostrobin. The sensitivity was improved by sweeping compare with common micellar electrokinetic chromatography method.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-51**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Three-phase direct immersion in-tube microextraction coupled with capillary electrophoresis

최지은 정두수*

서울대학교 화학부

Solid phase microextraction (SPME) and liquid phase microextraction (LPME) are widely used for sample enrichment and cleanup prior to an instrumental analysis. Compared to simply applicable SPME, LPME requires more manual maneuvers. In order to overcome such shortcomings of LPME, we developed in-tube microextraction (ITME). ITME uses a liquid plug inside a capillary as an acceptor phase and thus can be in-line coupled with capillary electrophoresis (CE) with ease. Since the acceptor phase is well protected inside the capillary, ITME can be carried out under severe extraction conditions. Moreover, given that the extraction and injection processes take place simultaneously, the extraction speed and efficiency are very high. Recently we have demonstrated headspace ITME by placing a separation capillary filled with an acceptor plug in the headspace above a sample solution using a commercial CE instrument. Here, we present 3-phase direct immersion ITME coupled with CE. By immersing the separation capillary containing a basic acceptor plug and a thin organic plug into an acidic sample solution, weakly acidic analytes in the neutral form are partitioned into the organic plug, and then back-extracted into the basic acceptor plug, followed by CE. With a 3-min extraction, Ketoprofen, Ibuprofen and Naproxen were enriched 975, 1100, and 1110 times, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL.P-52**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

SERS-based Wash-free Magnetic Immunoassay Using Sequential Droplet Merging and Splitting

최남현 고주희[1] 주재범[2,*]

한양대학교 바이오나노공학과 [1]한양대학교 나노센서연구소 [2]한양대학교 생명나노공학과

The combination of surface-enhanced Raman scattering (SERS) with microfluidic devices provides an ideal mechanism for achieving rapid, sensitive and reproducible detection of specific biomarkers in solution. An additional benefit of such platform is the use of minimal sample volumes and low analyte concentrations. We recently reported a SERS-based wash-free magnetic immunoassay technique using magnet-embedded droplet microfluidics. In this platform, the assay could be performed without any washing process by separating immunocomplexes from the supernatant solution using a magnetic separation. Nonetheless, this methodology still limited in assay because the channel structure for reagents injection and mixing is unified in a channel. To resolve this problem, a new class of microdroplet-merging device was designed and fabricated for sequential immunoassay. This device is composed of five distinct compartments such as droplets merging, separating immunocomplexes from supernatant solution, isolating magnetic immunocomplex droplets, and collecting unbound SERS probe droplets for detection. Herein, we report a novel SERS-based wash-free immunoassay device composed of compartments for mixing, merging, splitting and detection.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-53**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Novel Strategy for Quality Assessment of Glycosylation on a Biotherapeutic Glycoprotein by Intact Protein Analysis

김운용 오명진[1] 서영숙[2] 문한태[2] 안현주[2,*]

충남대학교 AGRS [1]충남대학교 분석과학대학원 [2]충남대학교 분석과학기술대학원

Protein glycosylation plays an important role in determining in vivo bioactivity, stability, solubility, and metabolic fate of biotherapeutics. Thus, detailed glycomic analyses are necessary complement to ensure quality, safety, and potency of therapeutic glycoproteins during production process. Current methods such as bottom-up and middle-down approaches employing LC-MS and LC-MS/MS for the glycomic characterization of biotherapeutics provide valuable information regarding glycan structure, isomers, and micro-heterogeneity. However, these methods significantly demand massive time and efforts from sample preparation to data interpretation. For these reasons, glycan or glycopeptide based approach is not suitable for real-time quality control in manufacturing processes. This study aims to develop novel analytical tool for real time determination of glycosylation site-occupancy with micro-heterogeneity using intact protein analysis (native mass spectrometry) without any additional sample preparation steps which can provide comprehensive glycosylation information.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-54**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Novel SERS-based Lateral Flow Assay Sensor for Rapid and Sensitive Detection of Autoantibody Against Citrullinated Peptide

전향아 이상엽[1] 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Rapid, user-friendly and versatile lateral flow (LF) strips have been extensively used for point-of-care (POC) and site-of-care (SOC) diagnostics. However, they have major limitations in terms of detection sensitivity and limited quantification capability. To resolve these problems, we recently developed a novel surface-enhanced Raman scattering (SERS)-based LF assay sensor for the quantitative analysis of a specific biomarker [1,2]. To assess the potential utility of SERS-based LF sensor in rheumatoid arthritis (RA) diagnosis, we extended the use of SERS-based LF assay platform to clinical samples of RA patients. In the first part of this work, the SERS-based LF assay for autoantibody against citrullinated peptide (anti-CCP) spiked in human serum was performed. For this purpose, CCP-immobilized LF strips and human IgG-conjugated SERS nano tags were prepared. Then the SERS signal of immunocomplexes on the test line was measured. Second, the SERS-based LF assay sensor was applied for real RA patient human sera collected by Hanyang University Hospital for Rheumatic Diseases. The clinical samples were divided into anti-CCP positive and anti-CCP negative groups according to their assay results by a commercially available ELISA kit. Next, the SERS-based LF assay results were compared to those measured by the commercially available ELISA kit. Statistical analyses were performed to evaluate the correlation between the ELISA and SERS-based LF assay results for both anti-CCP positive and negative patient groups.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-55**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Salivary Glycomic Approach for the Distinction of Human Constitutions

문한태 윤나영 김범진 안현주*

충남대학교 분석과학기술대학원

Unlike western medicine, oriental medicine has the constitutional diagnostics to determine individual health status. The accurate diagnosis of constitution is very important because therapy can be differed from patient’s constitution. Saliva, readily accessible and noninvasive fluid, contains mucins, which are heavily glycosylated proteins. Changes of glycosylation reflect health status because glycosylation is highly sensitive to the biochemical environment. In this study, we aim to conduct MS-based salivary glycomic approach to identify potential glycan signature for constitution classification. Saliva was collected from 9 normal people; 7 pancreotonia, 1 pulmotonia and 1 colonotonia. Initially, the saliva was filtered by 10K MWCO spin column to remove impurities. N-glycans were enzymatically released by PNGase F and purified by C18 SPE. Finally, the N-glycans were eluted by PGC SPE. For overall N-glycan profiling, both MALDI-TOF MS and nano-LC/Q-TOF MS were used to provide independent orthogonal analysis. Approximately 150 compositions of N-glycan were profiled and they were compared to identify the difference of glycans depending on presence (frequency), quantitation, composition, and structure. In constitution distinction, bi- and tri-antennary fucosylated N-glycans are high in abundance in pulmotonia and colonotonia while sialylated N-glycans are high in abundance in pancreotonia. MS-based salivary glycomic approach can be used as a discrimination system for the human constitution classification.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ANAL.P-56**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly Sensitive Detection of Estradiol Using SERS-based Competitive Immunoassay for the Diagnosis of Precocious Puberty

WANGRUI 전향아 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Estradiol (E2) is a biologically active sex steroid hormone that serves as important diagnostic marker in serum of premenopausal and postmenopausal women and in men. Particularly, the serum E2 concentration is very low (< 10 pg/mL) in prepubertal girls. In the past decades, several technologies, including high performance liquid chromatography-mass spectrometry (HPLC-MS), gas chromatography-mass spectrometry (GC-MS) and immunoassays have been developed for the measurement of E2. Unfortunately, current clinical detection methods are insufficient for accurate assessment of E2 at low concentrations (< 10 pg/mL). Thus, there is an urgent need for new technologies with efficient and sensitive detection of E2 for use in routine clinical diagnostics. In this study, we introduce a new E2 assay technique using a surface-enhanced Raman scattering (SERS)-based detection method. The SERS-based assay was performed with 30 blood samples to assess its clinical feasibility, and the limit of detection of E2 using the novel SERS-based assay described in this study was 0.65 pg/mL. Furthermore, this method showed a good correlation compared with the commercially available chemiluminescent microparticle immunoassay (CMIA) kit. Thus, the proposed SERS-based assay has a strong potential to be a valuable tool in the early diagnosis of precocious puberty due to its excellent analytical sensitivity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-57**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Simultaneous Detection of Dual Prostate Cancer Markers in Blood Serum Using SERS-Based Immunoassay

CHENGZIYI 주재범[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Prostate-specific antigen (PSA) is a 30-kDa serine protease. PSA in blood exists in dual forms; one is a free form and the other is a complexed form with the protease inhibitors a1-antichymotrypsin (ACT). Total PSA is a combination of both free and PSA/ACT complexed forms. Previous reports show that the clinical accuracy of PSA biomarkers can be improved by measuring the ratio between free-PSA and PSA-ACT in serum. In this work, we developed a novel SERS-based immunoassay technique for the simultaneous detection of both PSA/ACT and free-PSA biomarkers in serum. For this purpose, total-PSA antibody-conjugated magnetic beads and two different types of antibody-conjugated SERS nano-tags (MGITC labeled GNP conjugated with free-PSA monoclonal antibody (mAb) and XRITC labeled GNP conjugated with PSA/ACT mAb) were prepared. The assay was performed by the following procedure. First, total PSA antibodies were immobilized on the surface of a carboxyl-modified magnetic bead. Second, different ratios of PSA/ACT and free-PSA mixtures were prepared and added to the antibody-conjugated magnetic bead solution. Third, two different types of SERS nano-tags were added to the solution. Finally, the duplex sandwich immunocomplexes were isolated by a magnetic bar, and then the SERS signals of SERS nano-tags were measured and analyzed. This assay platform will be useful for the early diagnosis of prostate cancer patients.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-58**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Nano-Pillar Array Chip for the Rapid and Sensitive Detection of Food Poisoning Bacteria

고주희 박성규[1] 이상엽[2] 주재범[2,*]

한양대학교 나노센서연구소 [1]재료연구소 표면기술연구본부 [2]한양대학교 생명나노공학과

Rapid and sensitive identification of pathogenic bacteria is a key factor for the early diagnosis of infectious disease. Serological culturing-based assays are extensively used for the identification of bacteria but it takes a long time due to their culturing process. Polymerase chain reaction (PCR) is another analytical tool for detecting bacteria. However, PCR also needs an amplification of target genes using thermo-cycling steps because the concentration of target gene sequence is relatively lower than that of unrelated gene sequences. In many cases, amplification process causes false-positive signals and wrong identification. To resolve these problems, we developed a novel amplification-free SERS imaging sensor for the rapid and sensitive detection of Salmonella typhimurium bacteria. This technique does not require any cell culture or DNA amplification processes due to its highly sensitive detection capability. For this purpose, we fabricated antibody-conjugated SERS nano tags and three-dimensional nanopillar-pattered SERS substrates. The analytical strategy involves 3 steps; (1) immobilization of capture antibodies on nano-pillar substrate, (2) capturing of bacteria using specific interaction between antibodies and bacteria, and (3) labelling of bacteria with SERS nano tags and their SERS imaging detection. This SERS-based imaging sensor allows the limit of detection (LOD) of Salmonella typhimurium bacteria as low as 4,000 CFU/mL without any sample enrichment process. This SERS-based imaging technique is expected to be a potentially useful tool for the rapid and sensitive detection of pathogenic bacteria.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-59**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Application of Hansen solubility parameter to optimize extraction solvents of sample preparation methods

육한나 이민지 이성광*

한남대학교 화학과

Solubility parameter (SP) is an important physical and chemical properties for selecting a proper solvent. Both the total solubility parameter and its constituent partial solubility parameters(Hansen solubility parameters) are widely used for the selection of appropriate solvents for given solutes. The use of the solubility parameter for the selection of solvents is based on the well-known rule of chemistry: “like dissolves like.” Thus, if the intermolecular forces between the molecules of the solvent and between the molecules of a solute are of a similar strength, the solvent is usually a good solvent for this solute. In this study, we investigated the relation between solubility parameter of extraction solvent and that of analytes for sample preparation process such as solid phase extraction(SPE) and liquid-liquid extraction(LLE). The recoveries in a given system have been correlated by the difference between solubility parameter of solvents and that of analytes. This study will help to select optimum solvent for sample preparation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-60**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

QSPR studies for predicting the cloud point of nonionic surfactants

조승현 이민지 이성광*

한남대학교 화학과

Cloud point(CP) is the temperature above which aqueous solutions of non-ionic and zwitterionic surfactants become turbid. Cloud Point Extraction(CPE) is a separation and preconcentration procedure that has been extensively applied for trace metal and organic compound determination in agreement with the ‘‘green chemistry’’ principles compared to those extractions that use organic solvents. Considering the complexity of synthesis and CP measurement for nonionic surfactants, the optimization of CP determination is relatively tedious and time consuming. Thus, the computational approach becomes an ideal alternative for analyzing, interpreting, and predicting the properties of unknown molecules. This study aimed to predict cloud point of nonionic by using a quantitative structure-property relationship(QSPR) method. The data set of cloud point were collected from a series of 85 nonionic surfactants. The molecular descriptors in models were calculated by PreADMET program and dataset was divided into training and test set by using KNIME. The forward selection and bootstrap sampling method were applied to determine the optimum descriptor of the multiple linear regression(MLR) in RapidMiner. The performance of each model were compared with R^2 , RMSE(root mean square error), and MAE(mean absolute error) for training and test set. It was possible to know the applicable range of the prediction model by applicability domain(AD) of the results of each model. Y-scrambling was performed to confirm chance correlation of the model.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-61**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Simultaneous qualitative and quantitative analysis of polysaccharides by inverse gated decoupling ^{13}C Q-NMR spectroscopy

이정연 이태희[1] 이태곤[1] 이상원[*] 김종혁[1,*]

고려대학교 화학과 [1]한국화학연구원 화학분석센터

Quantitative nuclear magnetic resonance (Q-NMR) spectroscopy compared to liquid chromatography-mass spectrometry (LC-MS) is a useful technique for qualitative and quantitative analysis because standard reference is not required and a little amount of solvent is required. Signals of ^{13}C NMR spectrum are separated easier than ^{1}H NMR because ^{13}C NMR has a wide chemical shift (about 200 ppm for organics). These advantages result in high selection rate of a qualified signal and help quantitative analysis. However, ^{13}C NMR is proceeded by using power gated decoupling method, it makes Nuclear Overhauser Effect (NOE). Peak intensities were randomly increased and some errors of integrated peak were arisen by NOE. Inverse gated decoupling method was used to solve these problems because inverse gated decoupling minimizes the NOE and gets more accurate values. In this study, eight polysaccharides (sucrose, lactose, maltose, cellobiose, raffinose, melezitose, glucosamine, and galactosamine) were analyzed by inverse gated decoupling ^{13}C Q-NMR. The anomeric carbons of polysaccharides as the specific peaks were assigned to analyze qualitatively and quantitatively with maleic acid (20 mM, 129.99 ppm) which regarded as an internal standard in D2O. Influential factors, such as relax delay time (D1) and acquisition time (AT), were modified. As a real sample, cider beverage was analyzed qualitatively and quantitatively. The results showed that sucrose was included in the cider beverage. The chemical shift of sucrose was observed at 104.22 ppm when D1 was 10 sec and AT was 0.8 sec. Concentration of sucrose in cider beverage was 31.2 mg/mL and detection limits of polysaccharides were 50 mg/kg.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-62**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study on stability of lipid vesicle using asymmetrical flow field-flow fractionation (AsFlFFF) and dynamic light scattering (DLS)

김민욱 최재영 한수정 **Lars Nilsson**[1] 이승호*

한남대학교 화학과 [1]Lund University

Vesicles are of microscopic structure and composition that enclose a volume with a molecularly thin membrane. Generally the membrane is a self-directed assembly of amphiphilic molecules with a dual hydrophilic-hydrophobic nature, and is a spherical shell composed of lipid bilayer that encapsulate an aqueous space. Vesicles have been used as nano-scale containers for drugs, model membranes and other substances in pharmaceutical and cosmetic industries. Generally the stability of vesicles is closely related with their size and size distribution. When vesicles are used for drug delivery, the stability, and thus their life-time is directly associated with the medicinal effects. Thus size characterization of vesicles is necessary for understanding of the vesicle stability. Various techniques including electronic microscopy (EM), nuclear magnetic resonance (NMR), dynamic light scattering (DLS) and nanoparticle tracking analysis (NTA) have been used for size analysis of nano-sized particulates. DLS is simple to use, and has been widely used for analysis of particle size and its distribution. The application of DLS is however rather limited when dealing with samples of complex mixtures or of broad size distributions. Field-flow fractionation (FFF) has been employed for size-based separation and size-characterization of particles having broad size distributions from a few nm up to about 100 μm. Asymmetrical flow field-flow fractionation (AsFlFFF), one of members of FFF family, is particularly useful for characterization of aqueous colloidal particles.In this study, nano-sized vesicles were prepared by extrusion with the lipid concentration varied from 0.5 to 1.5%, and then were analyzed by AsFlFFF for determination of the size distribution, the stability (and life-time) and the osmotic pressure. It was found that the stability of vesicle increases as the lipid concentration increases. It was also observed that the vesicle stability is affected by the osmotic pressure.

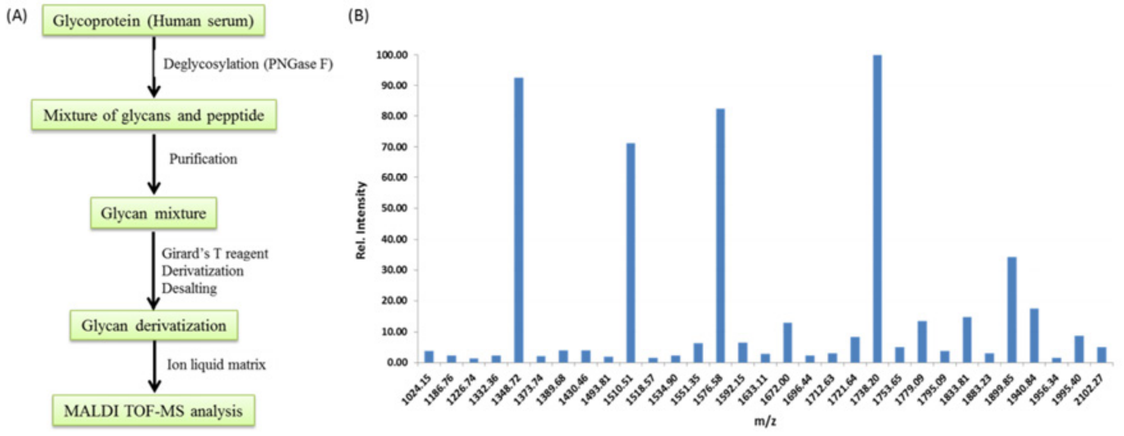
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-63**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Girard's reagent T derivatization and ionic liquid matrices for improved sensitive MALDI MS analysis of N-glycans

Le Thi Hoa 오동인[1] 강철훈[*] 김태우[*]

경희대학교 동서의학대학원 [1]경희대학교 의예과

Glycans are attached in glycoprotein and play important roles in biology, those are crucial for the development, growth, functioning, or survival of the organism. For enhanced mass spectrometry detection, N-glycans are often derivatized with some hydrazine reagents to form hydrazone products, which showed the usefulness for mass spectrometric analysis. Derivatization was introduced cationic site for detection of glycans by MALDI MS. In addition, ionic liquid matrices enhance homogeneous sample, thus leading to increase MALDI-MS intensity and reduced mass background. In this study, we investigated a new method to improve sensitive MALDI TOF-MS of N-glycans using ionic liquid matrices and Girard's T reagent derivatization.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-64**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study on the solvent clusters effect on Ionization efficiency of polycyclic aromatic hydrocarbons by Atmospheric pressure photoionization mass spectrometry

이슬기다운 김성환*

경북대학교 화학과

Analytical methods have been developed for the analysis of unknown compounds in accordance with the remarkable development of modern science and the specialization of analytical instruments. However, there still remain areas that cannot be clearly defined yet. Among them, there is a remaining challenge to identify and characterize the processes of ionization in mass spectrometry. One of the important process for the ionization is interaction between solvent cluster and analyte. In this study, the effect of solvent clusters exerted on the atmospheric pressure photo ionization of polycyclic aromatic hydrocarbons (PAHs) compounds were investigated. Eight molecules having similar molecular weight but different chemical structures were dissolved into various solvent compositions and ionization efficiencies were investigated. The obtained results were compared with thermodynamic parameters derived from theoretically calculated solvent clusters. Preliminary results show that methanol clusters lower sensitivity of analysis by reacting with toluene radical ions. In case of water cluster, the reactivity with toluene radical ions was lower and hence does not affect the ionization efficiency.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-65**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization of granule in egg yolk using asymmetrical flow field-flow fractionation (AsFlFFF) coupled with multiple detectors

한수정 최재영 Lars nilsson[1] 이승호*

한남대학교 화학과 [1]Department of Food Technology, Engineering and Nutrition, Lund University, Sweden

Egg yolk is used in various foods such as mayonnaise, salad dressing, baking, and custard cream. Egg yolk contains soluble proteins that are called ‘plasma’ and insoluble proteins that are called ‘granule’. The plasma of egg yolk is mainly composed of low-density lipoprotein (LDL) and livetin, while the granule is mainly composed of high-density lipoprotein (HDL), phosvitin and LDLg. LDL carries cholesterol from the liver to the tissue and cell, promoting the deposition of fat in the vessel. On the other hands, HDL (‘good cholesterol’) transports cholesterol out of tissues, promoting removal of excess cholesterol in the vessel. Granule is a complex mixture of HDL, phosvitin and LDLg. They are linked through the so-called ‘phosphocalcic bridge’, and are poorly soluble in water at neutral pH. Granules are dissociated at acidic or basic pH or at high ionic strengths. Thus, in food, granules have various degrees of dissociation and conformation depending conditions such as pH or the ionic strength. In this study, we studied on how the degree of dissociation or the conformation of granules change in mayonnaise using asymmetrical flow field-flow fractionation (AF4) coupled with multi-angle light scattering (MALS). The dissociated granule components were analyzed using sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-66**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Stable isotopic reconstructions of diets in Joseon Dynasty using human remains from archaeological site

강소영

국립문화재연구소 보존과학연구실

This study reports on human dietary reconstruction of Joseon Dynasty using stable isotope analysis. The stable carbon and nitrogen isotope values were measured of bone collagen extracted from 25 human bones from archaeological site in Myeongam-ri, Asan. Average values of $\delta^{13}C$ and $\delta^{15}N$ are –19.7±0.5‰ and 9.6±1.1‰ (n=23), respectively. The isotopic data indicates that Myeongam-ri individuals consumed C_3 plants mainly and assumed of dietary resourced from a terrestrial animal protein. Previous isotopic studies in Joseon period suggested that dietary composition of Joseon population was not influenced by region and burial type, but elevated $\delta^{15}N$ values in Mid-to-late Joseon era are attributed to consumption of resources from terrestrial animals. Also comparison of the isotopic results of male and female from double burials showed sex-dependent dietary patterns among individuals living in the same circumstances. These isotopic evidences have significance compared with dietary patterns of the Joseon population by various socio-economic factors and reconstruction of palaeodietary in Joseon Dynasty.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-67**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Determination of ceramides in human skins using UPLC/Q-TOF MS and /ultra-high resolution MS

박세민 서지영[1] 김영환*

한국기초과학지원연구원 생의학오믹스연구팀 [1]충남대학교 분석과학기술대학원

Ceramides (CERs) are mostly distributed in stratum corneum (SC) of skin epidermis layer and protect from noxious external environmental such as various allergen, pathogen and water evaporation. CERs are mainly composed of total 16 subclasses (Cer [NdS, NS, NP, NH], Cer [AdS, AS, AP, AH], Cer [EOdS, EOS, EOP, EOH], Cer [OdS, OS, OP, OH]) according to variable structure and chain length of fatty acid chain, sphingosine chain and polar head group. Above all, the SC of skin almost consists of N-type and A-type CERs. The analyses of CERs species have mainly used to normal-phase (NP) LC-APCI-MS with TLC method and reversed-phase (RP) LC/Q-TOF MS. To compare change of CERs species level between health skin and atopic dermatitis skin, we performed profiling and quantification of CERs in tape-stripped SC by RP-UPLC/Q-TOF MS, 15T FT-ICR MS and orbitrap MS. The use of XBridge BEH C18 Shield column (RP column), aminopropyl (NH_2) SPE cartridge and 7.5 mM ammonium acetate increased separation efficiency and ionization efficiency of CERs species. The acquired data was analyzed by principal component analysis (PCA) and orthogonal partial least square discrimination analysis (OPLS-DA) to investigate major alteration of CERs class by atopic dermatitis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-68**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Molecular characterization and comparison of Asphaltenes by APPI FT-ICR and Pyrolysis-GC/HRTOF MS

진장미 김성환[1] 김영환*

한국기초과학지원연구원 생의학오믹스연구팀 [1]경북대학교 화학과

Asphaltenes are complex mixtures with polar and nonpolar compounds and have high molecular weight. Especially, there are polyaromatic hydrocarbons with containing nitrogen, oxygen and sulfur in the raw carbon residue specimens. It is important to demonstrate molecular level characterization of asphaltenes because they raise problems in petroleum industry by their undesirable properties such as uncontrolled precipitation and aggregation. In this study, the molecular characterization of asphaltene has been investigated by APPI FT-ICR MS. The overall distribution of chemical classes was determined. As a result, it was observed that S_x, O_1S_1, O_1 and HC class species were abundant. Also, the double bond equivalents (DBE) versus carbon number plots were shown for detailed information. The raw carbon residue specimens were analyzed by Py-GC/HRTOF MS in order to identify their thermally decomposed constituents. Asphaltenes were thermally desorbed at 500℃ followed by another run at 800℃ without sample handling such as dissolution or filtration. The products of pyrolysis were also characterized by chemical class distribution and DBE versus carbon number plots for main class species.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-69**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Lipid mass fingerprinting of microorganisms by matrix-assisted laser desorption/ionization mass spectrometry

방글 김정아 김영환*

한국기초과학지원연구원 생의학오믹스연구팀

The rapid identification of bacteria is of increasing interest in food, biosafety, and clinical study. Due to rapid progress in the development of mass spectrometry devices and microorganism identification database during the last few years, bacteria identification by using mass spectrometry has become a very powerful and usable tool. We report a technique for rapid lipid profiling of bacteria by MALDI-TOF mass spectrometry. MALDI-TOF MS was applied to the rapid and direct detection of intact phospholipids from whole bacteria cells. The sample preparation procedure involved both depositing bacterial colonies directly onto the MALDI plate and using developed micro fluidic system. The phosphatidylethanolamines (PE) and phosphatidylglycerols (PG) in lipid mixture extracted from bacteria are observed in the MALDI-TOF mass spectra. The MALDI-TOF mass spectrum of each bacterial extract shows a distinguishing profile. In addition, the distinct discrimination of some species of gram negative bacteria was achieved by using principal components analysis (PCA) conducted on the relative peak intensities of phospholipids observed from the MALDI spectra. The experimental results demonstrate that the current technique is able of conducting rapid lipid analysis and has the potential for rapid clinical detection.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-70**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Graphite surface assisted laser desorption ionization time-of-flight mass spectrometry for small organic molecules

김민선 서정주 김정환*

한국기초과학지원연구원 질량분석장비개발팀

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry(MALDI TOF MS) has been proven as a particularly fast and effective tool for not only for the analysis of large molecules such as proteins and polymers but also for determination of small organic molecules. However, the detection of small organic molecules in MALDI TOF MS is screened by the common matrices and the inhomogeneous sample preparation is still remained one of major difficulties. Thus, matrix-free mass spectrometric techniques such surface-assisted laser desorption ionization mass spectrometry(SALDI) offer significant advantages for the analysis of small organic molecules.[1] Graphite plate is effective not only as an energy transfer medium like as a MALDI matrix but also as a sample substrate.[2,3] On graphite plate which has a hydrophobic surface property, sample preparation for hydrophobic materials is relatively easy and convenience to form homogenous sample surface, whereas hydrophilic materials such as amino acid and small peptide. In this study, we are demonstrated the SALDI TOF MS for small organic molecules using graphite plate as a sample substrate. Moreover, the sample preparation method for the hydrophilic materials is examined. The variety of application of graphite SALDI TOF MS will be discussed in detail. [1] Dattelbaum AM and Iyer S.,*Expert Rev Proteomics*., 2006, 3(1), pp. 153-61. [2] Junghwan Kim and Weekyung Kang., *Bull. Kor. Chem. Soc*., 2000, 21, pp. 401-404 [3] Kim and et. al., *Bull. Kor. Chem. Soc*., 2002, 23, pp. 315-319

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-71**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

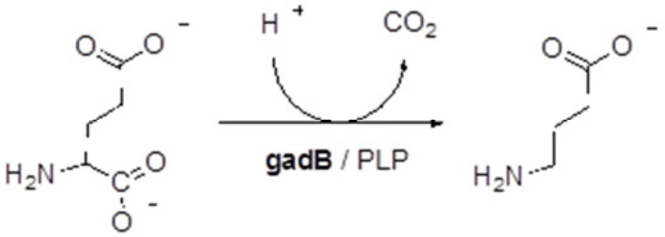
Study on oligomerization of glutamate decarboxylase (GAD) from *Lactobacillus brevis* (*L. brevis*) using asymmetrical flow field-flow fractionation with coupled multi-angle light scattering (AF4-MALS) and related techniques

최재영 Javier Linares-Pastén[1] Lars Nilsson[2,*] 이승호[*]

한남대학교 화학과 [1]Biotechnology, Department of Chemistry, Lund University [2]Department of Food Technology, Engineering and Nutrition, Lund University

Glutamate decarboxylase (GAD) catalyzes the decarboxylation of glutamic acid giving-aminobutyric acid (GABA) (figure 1). GAD uses pyridoxal phosphate (PLP) as co-factor and H^+ as co-substrate. This enzyme is broadly present in the living organisms, from bacteria to human. GABA is one of the main neurotransmission inhibitors in nervous central system. In addition, there is increasing interest of GABA because there are evidences that it can lower blood pressure in patients with mild hypertension[1] and other potential healthy beneficial effects[2], although these mechanisms are not known yet. GABA becomes an attractive potential functional ingredient for food, but the chemically synthesized GABA is not accepted for uses in food[3]. GABA was found in some fermented food, for instance Kimchi[4], and some strains of *Lactobacillus brevis* (*L. brevis*) were identified as ones of highly GABA producers[3]. In addition, *L. brevis* is recognized as putative probiotic due potential healthy effects in humans[5]. GAD from *L. brevis* and other lactic acid bacteria apparently play an important role in the low pH resistance since it uses protons in the GABA production. It was previously reported that the highest level of activity is reached when GAD is in hexameric form and lowest when is present as dimer[6,7]. Therefore, the oligomerization seems to play an important role in the GAD mechanism. In this work we have studied the effect of pH and salt concentration in the oligomerization of a recombinant GAD from *L. brevis*, using asymmetrical flow field-flow fractionation (AF4), dynamic light scattering (DLS) and molecular modeling methods.References1. Inoue, K., et al., Eur. J. Clin. Nutr., 57, 490-495 (2003)2. Li, H. and Cao, Y., Amino Acids, 39, 1107-1116 (2010)3. Wu, Q. and Shah N. P., Crit. Rev. Food Sci. Nutr., (2016)4. Cho,

Y. R., et al., J. Microbiol. Biotechnol., 17, 104-109 (2007)5. Yakabe, T., et al., Food Chem. Toxicol., 47, 2450-2453 (2009)6. Hiraga, K., et al., Biosci. Biotechnol. Biochem., 72, 1299-1306 (2008)7. Astegno, A., Et al., Biochim. Biophys. Acta, 1854, 1229-1237 (2015)



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

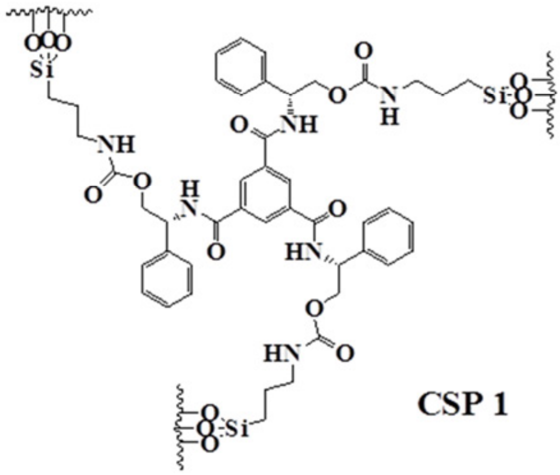
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-72**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and application of new (R)-phenylglycine and (S)-leucine derived C$_3$ symmetric HPLC chiral stationary phases

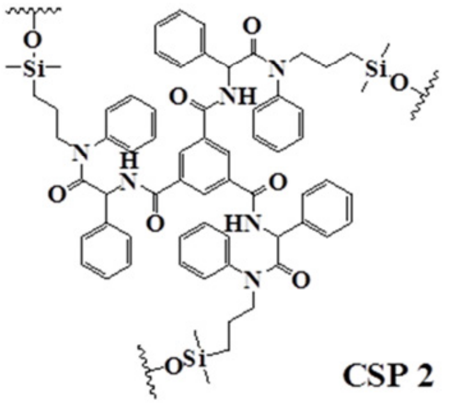
유정재 류재정[1,*]

경북대학교 화학과 [1]경북대학교 화학교육과

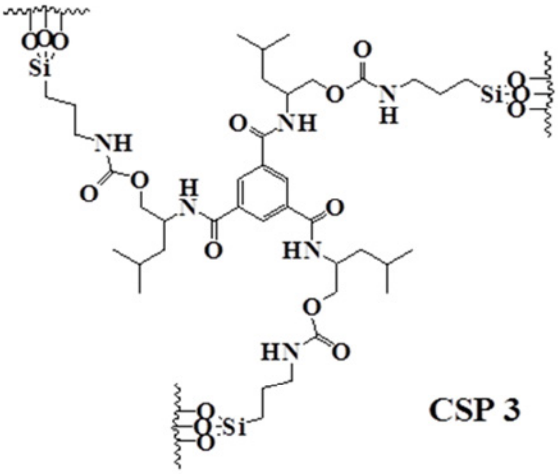
A new C$_3$ symmetric (R)-phenylglycinol *N*-1,3,5-benzenetricarboxylic acid derived chiral HPLC stationary phase (CSP 1) was reported recently and the CSP 1 showed good results in comparing with previously reported *N*-3,5-dintrobenzoyl(DNB) (R)-phenylglycinol derived CSP.[1] More than ten years ago, (S)-leucinol, (R)-phenylglycine and (S)-leucine derivatives were used for staring materials of 3,5-DNB based Pirkle type CSPs for chiral separation.[2,3] In this study, three C$_3$ symmetric CSPs(CSP 2, 3, 4) were newly prepared by the ideas and results of the three mentioned references.[1~3] The synthetic procedures and applications of the new C$_3$ symmetric CSPs (CSP 2 ~ CSP 4) will be shown.



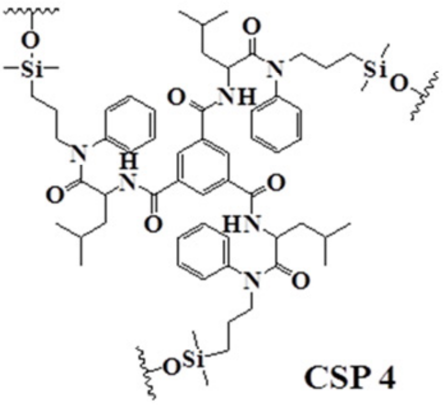
CSP 1



CSP 2



CSP 3



CSP 4

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ANAL.P-73**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of analysis methods of Benzisothiazolinone in cosmetic products by HPLC and LC-ESI-MS/MS

하서준

식품의약품안전청 식품의약품안전평가원/화장품연구팀

Benzisothiazolinone(BIT) is known for its function as antimicrobial agent. However, BIT is currently not listed in “Inventory; Ingredients which have authorized maximum concentrations" and "AnnexV" corresponding to list of preservatives allowed in Korea and EU respectively. Therefore BIT cannot be used as a preservative in cosmetics. Besides, BIT is moderately irritating to the skin and a moderate contact sensitizer. Accordingly it is important to prevent cosmetic products containing BIT as preservative by quality control (QC) methods.In this study, we have developed well qualified analysis methods for the determination of BIT in various cosmetic matrixes. These methods have been fully validated followed by "Korean pharmaceutical method validation guideline". Quantitative method was established by HPLC and identification was set up by LC-ESI-MS/MS. The coefficients of determination() were all greater than 0.999 in the range from 0.5 to 10.0 μg/mL for HPLC and 0.02 to 5.0 μg/mL for LC-MS/MS. They showed outstanding selectivity to the cosmetic matrixes. For HPLC method, the LOD and LOQ were calculated as 0.07 and 0.21 μg/mL. In the accuracy and precision test using skin, lotion, cream and shampoo matrixes, the average recovery rate was 99.75% and the relative standard deviation (RSD) was 0.33%. On the other hand, for the LC-MS/MS method, the LOD and LOQ were 0.01 and 0.03 μg/mL, and the accuracy and precision test results were 101.50% and 3.57% respectively. We expect that the results of this study can be usefully applied in QC of cosmetic products and contributed to improve consumer safety.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-74**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Measurement of sulfur mustard exposure by GC-TSQ analysis of TDG in human urine and plasma

김현석* 정창희[1] 이용한[2]

국방과학연구소 제5기술연구본부 [1]국방과학연구소 5기술본부 3부 [2]국방과학연구소 5본부 3부

Sulfur mustard is a vesicant agent that was developed in World War I for military purpose. Measurement of exposure to sulfur mustard is important for proper treatment and clear evidence presentation. In human body, sulfur mustard produces several metabolites including simple hydrolysis product thiodiglycol (TDG) and protein adducts. In this study, we focused on analysis of TDG in urine and plasma because protein adducts are also easily hydrolyzed to TDG using NaOH (aq). However, analysis of TDG is difficult due to its low concentration in urine and plasma as well as complex sample preparation. In this study, we tried to reduce sample preparation steps and analyze trace level of TDG through derivatization with MBTFA (*N*-methyl-*N*-bis(trifluoroacetamide)). Derivatized samples were successfully analyzed by using SRM (selected ion monitoring) mode of GC-TSQ.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-75**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Quantification of miRNA in a single cell using atomic force spectroscopy

구현서 박익범[1] 박준원*

POSTECH 화학과 [1]POSTECH 융합생명공학부

MicroRNA (miRNA) is short (~22 nt) non-coding single-stranded RNAs that play critical roles in controlling the expression level and regulate a variety of biological processes including cell apoptosis, proliferation, and development timing. Additionally, the abnormal regulation of miRNA is associated with a wide variety of human diseases such as cancers and neurological disorders. Thus, accurate quantification methods for miRNA detection with atomic force spectroscopy will lead us to understand miRNA mediated gene regulation at the single cell level with high lateral resolution of sub-nanometer. It is desirable to overcome the problematic limit, caused by the high similarity between pre-miRNA and miRNA during the force-based AFM experiment with high lateral resolution. Here, we demonstrate a new approach for the quantitative detection of miRNA without modification or amplification.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-76**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Visualization of Non-coding Cellular RNA in a Neuronal Cell Using Atomic Force Microscopy

박익범 구현서[1] 박준원[1,*]

POSTECH 융합생명공학부 [1]POSTECH 화학과

MicroRNAs (miRNA) are a class of short (19-25 nt) non-coding single-stranded RNA molecules that regulates in post-transcriptional gene expression. MiRNA controls the expression level of target proteins. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Detection of miRNAs has become an important emerging topic in biomedical fields. Therefore, accurate quantification of miRNAs from biological samples will lead us to better understanding of the role of miRNAs. Conventional methods widely used in the detection of miRNAs mainly include northern blotting, microarray, real-time RT-PCR and in-situ hybridization. Especially, In situ detection of intracellular miRNAs requires simple sample preparation, without cell lysis and RNA isolation, and provides additional information on the subcellular localization of miRNAs. However, conventional tools are not easy to detect high spatial localization and sensitive detection of miRNAs. Therefore, a new approach for miRNA detection tool is atomic force microscopy (AFM). AFM has been extensively used to observe interaction of molecules and manipulate biomolecules in the physiological conditions at the single-molecule level. Because AFM has high lateral resolution of sub-nanometer, the nanoscale distribution of individual molecules on the sample surface could be imaged. Here, we established an AFM-based miRNA quantification and distribution method with no requisite of labeling for modification of miRNAs. In this research, the detection of a specific miRNAs in a cultured neuronal cell is measured by force-based AFM and help to understand functions of miRNA in depth.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-77**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rhamnetin Exhibits Anti-Tuberculosis Activity and Protects against Lung Inflammation

김민준 전다솜 김양미*

건국대학교 생명공학과

Rhamnetin, a natural flavonoid found in cloves and berries has been reported to show anti-inflammatory activities in lipopolysaccharide-stimulated RAW264.7 cells and may be a potent inhibitor for extracellular signal-regulated kinase 1 (ERK1) and c-Jun N-terminal kinase (JNK). Here, we showed that rhamnetin has antimycobacterial effects on Mycobacterium tuberculosis (MT) H37Rv, multi-drug-, and extensively drug-resistant clinical isolates. We also investigated the effect of rhamnetin on interferon (IFN)-γ-stimulated human lung fibroblast MRC-5 cells, since MT infection causes intensive lung inflammation. Rhamnetin suppressed mRNA levels of tumor necrosis factor-α, interleukin (IL)-1β, IL-6, IL-12, and matrix metalloproteinase-1. Furthermore, it inhibited IFN-γ-mediated stimulation of ERK1 and p38 mitogen-activated protein kinase in MRC-5 cells. These results showed that rhamnetin has potent anti-tuberculosis activities and effectively suppresses lung inflammation, implying that rhamnetin can be a potent anti-tuberculosis dietary agent.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-78**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Papiliocin as a Potent Peptide Antibiotic against Gram-Negative Bacteria

전다솜 김양미*

건국대학교 생명공학과

A novel 37-residue, cecropin-like peptide, papiliocin, isolated from the swallowtail butterfly Papilio xuthus, possesses high bacterial cell selectivity, particularly against gram-negative bacteria. To understand structure-activity relationships, we determined the 3-D structure of papiliocin in 300mM DPC micelles by nuclear magnetic resonance (NMR) spectroscopy, showing that papiliocin has an α-helical structure from Lys3 to Lys21 (N-terminal helix) and from Ala25 to Val36 (C-terminal helix), linked by a hinge region. Interactions between the peptides and lipids were studied using saturation transfer difference-NMR experiments and MD simulation. The results imply that the Trp2 and Phe5 in the amphipathic N-terminal helix are important in the rapid permeabilization of the gram-negative bacterial membrane. The hydrophobic C-terminal residues permeabilize the hydrophobic bacterial cell membrane synergistically with these aromatic residues, providing selectivity against gram-negative bacteria. We measured the anti-inflammatory activities of papiliocin against gram-negative bacteria in vitro and in vivo, implying that papiliocin can be a potent peptide antibiotic for the therapeutic application.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-79**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A dietary flavonoid exerts anti-tuberculosis activity and suppresses lung inflammation

전다솜 정민철 김양미*

건국대학교 생명공학과

Phloretin found in apples and berries is known to have anti-oxidative and anti-cancer activities. In this study, we demonstrated that phloretin has anti-tuberculosis activities against Mycobacterium tuberculosis H37Rv, multi-drug- and extensively drug-resistant clinical isolates. Mycobacteria cause lung inflammation that contributes to tuberculosis pathogenesis. We evaluated the anti-inflammatory effects of phloretin in interferon (IFN)-γ-stimulated MRC-5 human lung fibroblasts and LPS-stimulated dendritic cells as well as in vivo mouse model. Release of interleukin (IL)-1β, IL-12, and tumor necrosis factor (TNF)-α was inhibited by phloretin and the mRNA levels of IL-1β, IL-6, IL-12, TNF-α, and matrix metalloproteinase-1 as well as p38 mitogen-activated protein kinase and extracellular signal-regulated kinase phosphorylation were suppressed. These results implied that phloretin is able to permeabilize the M. tuberculosis cell membranes and can be a useful dietary supplement with anti-tuberculosis benefits. We will discuss about the candidate target proteins of anti-TB activities of phloretin.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-80**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Structure and Dynamics of Mesophilic and Thermophilic Acyl Carrier Proteins

정민철 이영준[1] 김양미*

건국대학교 생명공학과 [1]건국대학교 생명특성화대학

Acyl carrier protein (ACP) is an important cofactor in biosynthetic pathways in the type II fatty acid synthesis (FAS) system. Since interactions between ACP and FAS enzymes are critical, the conformational changes and the loop motions of ACP are responsible for reversible interaction with them. We have investigated the structures of ACP from mesophilic and thermophilic bacteria. All ACPs have a conserved aromatic residue at the end of helix II whereas E. faecalis-ACP (Ef-ACP) has an additional Phe (F45) and hyperthermophilic T. maritima-ACP (Tm-ACP) has an additional Phe (F50) in the middle of helix II. Despite high similarities between E.coli-ACP (Ec-ACP), Ef-ACP, and Tm-ACP, the melting temperatures are markedly different from each other. Extensive network of ionic clusters in Tm-ACP is the key factors for the extremely high thermal stability of Tm-ACP while hydrophobic interaction between F45 in helix II with F18 in the α1α2 loop and a hydrogen bonding between S15 in helix I and I20 in the α1α2 loop is the key features for the thermal stability of Ef-ACP. Furthermore, we investigated the dynamics of these ACPs and the relationships between their structural flexibilities and the thermal stabilities are compared. Since multi-drug resistant gram-negative bacterial infections are threatening worldwide, we tried to discover new antibiotic compounds that have novel mechanisms toward target enzyme, β-ketoacyl-(acyl carrier protein) synthase III (KAS III). We performed receptor-oriented pharmacophore-based in silico screening of E.coli as well as A. baumannii KAS III. We identified potent KAS III inhibitors with antibacterial activities against gram-negative bacteria. Further optimization of this compound is required to improve its antimicrobial activity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-81**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Structure and dynamics of *Propionibacterium acnes* Acyl Carrier Protein studied by NMR spectroscopy

천다솜 정민철 김양미*

건국대학교 생명공학과

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 (ACP) is an essential part of its FAS. In this study, P. acnes ACP was cloned and 15N and 13C labeled protein was expressed and purified. We performed 3D NMR experiments and completed backbone assignment. P. acnes ACP has four • •helices (• 1 (I7-T19), • 2 (S40-F54), • 3 (D60-N65), and • 4 (V69-H79)). Using CD spectra, the melting temperature of P. acnes ACP was determined as 56°C, which is much lower than those of other ACPs, implying its low thermostability. We also discovered a potent inhibitor for the P. acnes FAS protein as a novel antibiotic against P. acnes infection as well as anti-inflammatory agents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-82**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Important Structural Features of the Psychrophilic Cold-Shock Protein from Colwellia psychrerythraea, Studied by Nuclear Magnetic Resonance Spectroscopy

이영준 정민철[1] 김양미[1,*]

건국대학교 생명특성화대학 [1]건국대학교 생명공학과

Cold-shock proteins (Csps)—proteins expressed when ambient temperature drops below growth-supporting temperature—bind to single-stranded nucleic acids and act as RNA chaperones to regulate translation. Colwellia psychrerythraea is an obligate psychrophile, Gram-negative bacteria found in continually cold marine environments including arctic and antarctic sea ice. Despite dramatic differences in the thermostability of Csps of various thermophilic microorganisms, CSPs share high primary sequence homology and a high degree of three-dimensional structural similarity. C. psychrerythraea Csp (Cp-Csp) is less thermostable with a lower melting temperature (38℃) compared with mesophilic and thermophilic Csps. Here, we investigated the structural and dynamic feature of Cp-Csp. Cp-Csp has a five-stranded β-barrel structure with hydrophobic core packing. The structural flexibility that accompanies longer surface loops and less hydrophobic core packing as well as a number of salt bridges are likely key factors in the low thermostability of Cp-Csp. This implies that the large conformational flexibility of psychrophilic Cp-Csp, which more easily accommodates nucleic acids at extremely low temperature, is required for RNA chaperone function under cold-shock conditions and for the cold adaptation of C. psychrerythraea.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-83**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Construction of hydrocarbon stapled cell-penetrating peptides to deliver short RNAs

현순실 이연[1] 유재훈*

서울대학교 화학교육과 [1]서울대학교 화학부

In spite of various kinds of cell penetrating peptides have been developed for noncovalent-based delivery of short interfering RNAs, micromolar concentrations are usual dosage for full penetrating ability and efficient delivery. At these high concentrations, the cell penetrated peptides could inhibit intracellular targets and the over-dosed short RNAs might give off-target effects. To reduce cyto-toxicity and off-target effects, cell penetrating capacity of peptides should be improved. We recently prepared position specific stapled peptides, among which a His containing stapled cell penetrating peptide was selected as siRNA delivery tool. LKH stEK showed the best siRNA delivery potential, affording significant uptake of siRNA even at less than 6 nM concentrations. We also found that the target gene was 90% knock downed with 2.5 μM concentration of the peptide and 50 nM of siRNA. Since LKH stEK has negligible cytotoxicity even at 20-fold higher concentration used for siRNA delivery, the specificity of target gene knock down is guaranteed. Taken together, low nanomolar siRNA can be delivered to eukaryotic cells efficiently by simply complexing with stapled cell penetrating peptide and LKH stEK mediated siRNA delivery into mammalian cell induces target knockdown.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-84**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Non-hemolytic cell penetrating peptides: site specific introduction of glutamine and lysine residues into an α-helical peptide causes deletion of its direct membrane disrupting ability but retention of its cell penetrating ability

현순실 이연[1] 유재훈*

서울대학교 화학교육과 [1]서울대학교 화학부

Cationic and amphipathic characters of α-helical peptides are commonly found in cell penetrating peptides (CPPs). These features give CPPs both membrane demolishing and penetrating abilities. Safe biomedical applications of CPPs require that toxicities resulting from their membrane demolishing abilities be removed while their cell penetrating abilities be retained. In this study, we systematically constructed mutants of the amphipathic α-helical model peptide (LKKLLKLLKKLLKLAG, LK peptide). The hydrophobic amino acid leucine in the LK peptide was replaced by hydrophilic amino acids in order to reduce hemolytic or cell toxicity. Most of the mutants were found to have reduced membrane disrupting abilities but their cell penetrating abilities were also decreased. However, importantly, L8Q and L8K mutants were found to retain their cell penetrating abilities in the low micromolar range and to lose their membrane disrupting ability almost completely. These selected mutants utilize energy-dependent endocytosis mechanisms instead of energy-independent direct cell penetrating mechanism to enter into cells. In addition, the mutants can be used to successfully deliver the anticancer drug, methotrexate (MTX), into cells to overcome the drug resistance. To determine if the mutation effect on the membrane disrupting ability and cell penetrating ability is general, Q and K mutations of the natural amphipathic α-helical antimicrobial peptide (AMP), LL37, were carried out. Specific positional Q and K mutants of LL37 led to lower hemolytic toxicity effectively while preserving its cell penetrating ability to eukaryotic cells such as MDA-MB-231. Taken together, observations made in this effort suggest that interrupting the global hydrophobicity of amphipathic α-helical CPPs and AMPs by replacing

hydrophobic residues with mildly hydrophilic amino acids such as Q and K might be an ideal strategy for constructing peptides that yield high cell penetrating abilities without disrupting membranes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-85**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of paralleled and anti-paralleled oriented dimer bundle of amphipathic α-helical peptides by two disulfide bonds and their cell penetrating ability

현순실 이연[1] 유재훈*

서울대학교 화학교육과 [1]서울대학교 화학부

α-Helical amphipathic peptides with cationic residues generally possess cell penetrating ability against eukaryotic membrane at their micromolar concentrations. Recently, our laboratory demonstrated that the formation of a disulfide dimeric bundle with a model LK peptide acquires unusually high cell penetrating ability, affording almost quantitative translocation of eukaryotic membrane at their low nanomolar concentrations. In this study, we further modify this model peptide in different orientations to elucidate the nature of the cell penetrating ability. We synthesized separately paralleled and antiparalleled dimers using different side chain protecting groups of Cys monomer, Trt and Acm. Flow cytometry analysis showed that the cell penetrating ability of the air oxidized dimer is almost identical with that of antiparalled dimer. The helicity measurement using a circular dichroism spectrometer confirmed that the antiparalleled dimer has more alpha helical propensity than the paralleled dimer. It was also found that the alpha helical conformation of the air oxidized dimer resembles that of antiparalleled dimer. These data suggest that the intermolecular hydrophobic interactions lead the stable orientation of the dimer bundles, which is essential for the cell penetrating. Potent cell penetrating peptides against eukaryotic membrane could be designed by applying these newly found observations.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-86**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mechanistic diversification and spin state variation of rice allene oxide synthase-1 by site-directed mutation at Phe-92 and Pro-430

한옥수

전남대학교 분자생명공학과

Allene oxide synthase (AOS) and hydroperoxide lyase (HPL) are members of cytochrome P450 subfamily 74 (CYP 74) which is classified as a non-classical cytochrome P450 since they do not require molecular oxygen or NADPH-dependent P450 reductase for their activities. The magnitude of spectral shift induced by imidazole binding was linearly co-related with the partial inhibition of OsAOS1 activity of using HPODE as a substrate. The spectral shift indicates that imidazole may coordinate to ferric heme iron, triggering a heme-iron transition from high spin state to low spin state. In order to clarify relationship between spectral shift and relative partitioning of activities between allene oxide synthase and hydroperoxide lyase, F92 and P430 of OsAOS1 were selected for point mutations. Partition ratio for HPL activity was increased by F92L mutation with the partial shift of Soret maximum toward 424 nm. P430A mutation also shifted the Soret maximum toward 424 nm. Double mutation (F92L/P430A) of OsAOS1 increased the partition ratio for HPL activity with the expected spectral shift. Therefore, the structural variations of OsAOS1 by binding of Type II ligands and point mutations at F92 and P430 manipulated the partition of OsAOS1 between for AOS and HPL activities. Our results imply that the spin state of OsAOS1 is an important determinant to functionally separate AOS from HPL pathway of OsAOS1 reaction or CYP74 in general, requiring high spin for AOS activity and low spin for HPL activity, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-87**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Immobilization of lipoxygenase on nanoporous rice husk silica by adsorption and production of hydroperoxy fatty acids

한옥수

전남대학교 분자생명공학과

Lipoxygenase catalyzes the conversion of polyunsaturated fatty acids (PUFA) into hydroperoxy fatty acids. The synthesis of hydroperoxy fatty acids is the first committed step of oxylipin biosynthesis in plants. Hydroperoxy derivatives of PUFA are important molecules due to their biological functions in plant defense. The immobilization of LOX enzyme in solid-supports is crucial for the industrial production of hydroperoxy fatty acids. In this study, soybean LOX was immobilized on nanoporous rice husk silica (RHS) by using nonspecific adsorption method, and the immobilized enzymes' properties were characterized. The amount of RHS-adsorbed soybean LOX was increased in proportion to the total amounts of soybean LOX and RHS and at least 30-35 % was adsorbed nonspecifically. RHS-adsorbed soybean LOX maintained 73 % of free soybean LOX activity. Dissociation kinetics of RHS-adsorbed soybean LOX indicated that the amount of dissociated RHS–adsorbed soybean LOX reached to the saturation after 3 months. The optimal pH for nonspecific adsorption of soybean LOX on RHS was 7.04, while the optimal reaction temperature was 60 oC for both free and RHS-adsorbed soybean LOX. RHS-adsorbed soybean LOX could be repeatedly used for at least 4 cycles, and nearly 59 % of the initial activity was retained even after the 5 cycles. Collectively, nanoporous rice husk silica (RHS) was found to be a suitable matrix for the direct, simple, rapid, and less expensive immobilization of soybean LOX.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-88**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Protective effect of recombinant soluble neprilysin against b-amyloidinduced neurotoxicity

오재훈

서울대학교 화학부

A few decades ago, researchers found emerging evidence showing that a number of sequential events lead to the pathological cascade of Alzheimer's disease (AD) which is caused by the accumulation of amyloid beta (Ab), a physiological peptide, in the brain. Therefore, regulation of Ab represents a crucial treatment approach for AD. Neprilysin (NEP), a membrane metallo-endopeptidase, is a rate-limiting peptidase which is known to degrade the amyloid beta peptide. This study investigated soluble NEP (sNEP) produced by recombinant mammalian cells stably transfected with a non-viral NEP expression vector to demonstrate its protective effect against Ab peptides in neuronal cells in vitro. Stably transfected HEK 293 cells were used to purify the soluble protein. sNEP and Ab peptide co-treated hippocampal cells had a decreased level of Ab peptides shown by an increase in cell viability and decrease in apoptosis measured by the CCK-8 and relative caspase-3 activity ratio assays, respectively. This study shows that stably transfected mammalian cells can produce soluble NEP proteins which could be used to protect against Ab accumulation in AD and subsequently neuronal toxicity. Additionally, approaches using protein therapy for potential targets could change the pathological cascade of Alzheimer's disease.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-89**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Structural Elucidation of Syndecan-4 Receptor with NMR Spectroscopy

김지선 최성섭 김용애[*]

한국외국어대학교 화학과

Syndecan-4 consists of heparan sulfate proteoglycans which are present on the surface of all cell types in humans. It provides a mechanical link among the extracellular matrix and the actin cytoskeleton via binding interactions of its cytoplasmic tail. It also interacts with numerous binding partners and initiates a wide range of signaling processes and regulates diverse physiological processes like wound healing, arterial development, blood pressure regulation, immunosuppression and protection from endotoxic shock. To get a better understanding of the mechanism and function of syndecan-4, it is crucial to investigate its three dimensional structure.Syndecan-4 comprises three major sections: extracellular (ecto-), transmembrane (TM) and cytoplasmic (Cyto-) domains. The cytoplasmic domain of syndecan-4 consists of 28 amino acids and includes V domain. The binding of PIP2 at V domain of syndecan-4 causes the structural change of whole cytoplasmic domain of syndecan-4 and this leads binding and activation of PKC-α. Thus, the structural alteration of the transmembrane and cytoplasmic domains by binding with PKC-α and PIP2 regulates the function of the extracellular domain.Here, we optimize recombinant production processes of syndecan-4 that contain wild type Syd4-TM (wtSyd4), mutant Syd4-TM(mSyd4) and Syd4-eTC(ecto-, TM, Cyto-). The expression and purification processes of three Syd4 proteins were optimized. And its structure was investigated by SDS-PAGE, CD spectroscopy, mass spectrometry and solution/solid-state NMR spectroscopy. Optimized 3D structures of Syd4 based on 2D SAMPI4 solid-state NMR were confirmed by Molecular Dynamics Simulation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-90**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

NMR structural analysis of disease related human transmembrane proteins

조성진 김지선 김용애*

한국외국어대학교 화학과

Transmembrane proteins have a important role in biological processes, as they are involved in ion transport, channel formation, signaling and cell to cell interaction. In human cells, they are commonly targets for pharmaceuticals. Despite their importance, structural and functional studies of transmembrane proteins have been a difficult task due to the membranous properties and limited amount of material available. So, it remains a lack of biophysical and structural data.We tried to obtain large quantities of the amyloid-β (hAβ) that is related to the dementia and human melanocortin-4 receptor (hMC4R) that is related to the severe early onset obesity for biophysical and structural studies of disease related human transmembrane proteins. The hAβ transmembrane protein shows that the non-fibrillar hAβs form the Ca2+-permeable ion channel in the cell membrane and these channels can disrupt the normal cellular calcium homeostasis. It plays an important role in pathogenesis of dementia and Alzheimer disease. The hMC4R is located primarily in the brain and regulatory role in food intake and energy homeostasis. Heterozygous mutation D90N located in second transmembrane domain of hMC4R results in human obesity, hyperphagia and insulin resistance.In this research, we succeed to produce the transmembrane domain of the hAβ and second transmembrane domain of hMC4R. Structural characterizations of these proteins in the membrane environments were obtained by 1D/2D solution and solid-state NMR spectroscopy. We also present the optimized design, construction, and efficiency of a home-built 800 MHz narrow-bore (NB) 1H-15N solid-state NMR probe. 1H-15N 2D SAMPI4 spectra from membrane proteins in oriented bicelles were successfully obtained by using these solid-state NMR probe.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-91**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Method Development for Metabolomics of Phosphatidyl Inositol Derivatives in Live Cells under Different Conditions

이관호 채우리 유병용[1] 하상수*

경희대학교 화학과 [1]한국과학기술연구원(KIST) 특성분석센터

A highly sensitive quantitation method based both on the conventional HPLC and accelerator mass spectrometry (AMS) for intracellular mass distribution studies of phosphatidyl inositol (PI) derivatives is presented. PI derivatives are a class of phospholipids, derived from a parental molecule of inositol. They play important roles as precursors or second messengers for cell signaling processes such as hormone-dependent signal transduction. Their various and unique roles in cell signaling processes are mainly dependent on the locations and/or the number of phosphate groups. In this study, cells were dosed with 14C-inositol under different conditions, and PI derivatives mixed with other lipid components were obtained from the cells via the conventional extraction procedures, followed by HPLC separation and AMS measurements. 14C/12C ratios of each HPLC fraction were measured, revealing the mass distribution of the PI derivatives in cells under the given conditions. HPLC-based separation and AMS-based quantitation of the PI derivatives in cells for the phosphoinositide-related metabolomics (i.e. lipidomics) may contribute to drug development for pharmaceutical therapy of lipid-related diseases, because the profile of theintracellular PI derivatives and/or their mass distribution in tissue can be correlated with the cells' status. Our AMS-based method is an alternative or superior to the conventional 32P-based method for quantitation of intracellular PI derivatives.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-92**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Bioorthogonal Click Chemistry-Based Synthetic Cell Glue

구희범* 손지환[1] 윤석현[2]

가톨릭대학교 의과대학/의생명과학교실 [1]가톨릭대학교 의생명건강과학과 [2]Harvard Medical School & Massachusetts General Hospital

Artificial methods of cell adhesion can be effective in building functional cell complexes in vitro, but methods for in vivo use are currently lacking. Here, a chemical cell glue based on bioorthogonal click chemistry with high stability and robustness is introduced. Tetrazine (Tz) and trans-cyclooctene (TCO) conjugated to the cell surface form covalent bonds between cells within 10 min in aqueous conditions. Glued, homogeneous, or heterogeneous cell pairs remain viable and stably attached in a microfluidic flow channel at a shear stress of 20 dyn cm−2. Upon intravenous injection of assembled Jurkat T cells into live mice, fluorescence microscopy shows the trafficking of cell pairs in circulation and their infiltration into lung tissues. These results demonstrate the promising potential of chemically glued cell pairs for various applications ranging from delivering therapeutic cells to studying cell–cell interactions in vivo.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-93**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Sturctural studies of STAM-binding protein, AMSH as Ubiquitin Detaching Enzyme

정양욱 송현규[1,*]

고려대학교 생명과학과 [1]고려대학교 생명과학부

Ubiquitination (or Ubiquitylation) is an enzymatic post-translational modification in which the last residue of Ub, glycine, is covalently attached to a lysine residue of substrate proteins. Enzymes known as deubiquitinating enzymes (DUBs) can remove Ub bound to protein and regulate the temporary activity of Ub. Ub bound proteins are processed in several ways depending on the type of Ub binding. As one of non-proteasomal functions, monoubiquitination and K63-Ub implicate in the initiation and elongation of endocytosis in yeast, respectively. One of the well-characterized deubiquitinating enzymes is AMSH (associated molecule with the SH3 domain of STAM). AMSH consists of an N-terminal MIT domain (residues 11-110), a clathrin binding domain (CBD, residues 134-171), a middle coil region containing a single consensus P-X-V/I-D/N-R-X-X-K-P (RxxK) peptide motif, which interact with SH3 domain of STAM, and a C-terminal catalytic JAMM (JAB1/MPN/Mov34) domain. Previously, the crystal structures of C-terminal JAMM and N-terminal MIT domain have been reported by two independent groups, however the relative orientation of these domains and regulation of deubiquitinating activity by the other domains remain obscure. We have intensively investigated the structure of full-length AMSH with crystallography, although we couldn't make well-diffracted crystals yet. Here, we present the results of structural studies on AMSH performed with solution scattering, SEC-MALS, cross-linking, and molecular simulation. Successful data can build globular structure of target protein, which enable to elucidate the whole structure of full length AMSH.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-94**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

ACCORD: an assessment tool for the determination of coiled-coil orientation

<u>김병원</u> 정양욱 김민경[1] 오선주 송현규[1,*]

고려대학교 생명과학과 [1]고려대학교 생명과학부

The coiled-coil (CC) domain is a very important structural unit of proteins and plays critical roles in various biological functions. The major oligomeric state of CCs is a dimer, which could either be parallel or antiparallel. The orientation of each • •helix in a CC domain is critical for the molecular function of CC-containing proteins but cannot be determined easily using sequence-based prediction. We developed a biochemical method for assessing differences between parallel and antiparallel CC dimers and named it ACCORD (Assessment tool for Coiled-Coil ORientation Decision). To validate this technique, we applied it to 13 different CC proteins with known structures. Furthermore, the ACCORD was able to accurately determine the orientation of a CC domain of unknown directionality, which was confirmed by X-ray crystallography and small angle X-ray scattering. The ACCORD can be used as a general tool to determine CC directionality to supplement in silico prediction results.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-95**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The structure and biochemical analysis of yeast N-terminal amidase (Nta1), involved in the first step of N-End Rule Pathway

김민경 오선주[1] 송현규[*]

고려대학교 생명과학부 [1]고려대학교 생명과학과

The first step of the hierarchically organized N-end rule pathway of protein degradation is deamidation of the N-terminal glutamine and asparagine residues of substrate proteins to glutamate and aspartate, respectively. These reactions are catalyzed by the N-terminal amidase (Nt-amidase) Nta1 in fungi such as Saccharomyces cerevisiae, and by the glutamine-specific Ntaq1 and asparagine-specific Ntan1 Nt-amidases in mammals. To investigate the dual specificity of yeast Nta1 (yNta1) and the importance of second-position residues in Asn/Gln-bearing N-terminal degradation signals (N-degrons), we determined crystal structures of yNta1 in the apo state and in complex with various N-degron peptides. Both an Asn-peptide and a Gln-peptide fitted well into the hollow active site pocket of yNta1, with the catalytic triad located deeper inside the active site. Specific hydrogen bonds stabilized interactions between N-degron peptides and hydrophobic peripheral regions of the active site pocket. Key determinants for substrate recognition were identified and thereafter confirmed using structure-based mutagenesis. We also measured affinities between wild-type yNta1, its mutants and specific peptides, and determined KM and kcat for peptides of each type. Together, these results elucidate, in structural and mechanistic detail, specific mechanisms in the first step of the N-end rule pathway.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-96**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Role of p53 in senescence of normal human fibroblasts

김혜정 김문무*

동의대학교 화학과

Cellular senescence plays an important role in human aging. In particular, aging is the process related to the accumulation of molecular damage by reactive oxygen species (ROS). In particular, hydrogen peroxide (H_2O_2), by-product of mitochondrial respiration, is potential major inducer of oxidative damage and mediators of aging. In this study, we investigated the expression of genes and proteins on both in normal human lung fibroblast and in aged cells induced by H_2O_2. Firstly, SA-*β*-galactosidase staining, an aging marker was examined in young and aged cells induced by H_2O_2. Hydrogen peroxide treatment at 500μM showed the highest SA-*β*-galactosidase staining. Secondly, the expression of genes and proteins was analyzed in both normal young cells and old human lung fibroblasts. Lastly, the expression of genes and proteins was analyzed in both young and aged cells induced by H_2O_2. The expression levels of *p*-p53 and *p*-p21 were increased in normally aged cells. In addition, the expression levels of *p*-p53 and *p*-p21 were increased in aged cells induced by H_2O_2 at 500μM. These results suggest that the activation of p53 could modulate aging mechanism.Key words : Aging, p53, Human fibroblasts, Hydrogen peroxide(H_2O_2)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-97**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

β-Caryophyllene Oxide Inhibits PMA-induced MMP-2 and MMP-9 Activities in Human fibrosarcoma Cells

홍수경 김문무*

동의대학교 화학과

β-Caryophyllene oxide (CPO) has been reported to have not only bioactivity such as anti-inflammatory and immune activitise but also inhibition of growth and induction of apoptosis in tumor cells. CPO is a sesquiterpene isolated from essential oils of medicinal herbs with aroma such as guava leaves, oregano, cinnamon and black pepper. The purpose of this study is to investigate an inhibitory effect of CPO on matrix metalloproteinases (MMPs) that play an important role in tumor cell invasion using human fibrosarcoma cells (HT1080). First of all, the effect of CPO on cell viability in HT1080 cells was observed using MTT assay. Its cytotoxicity was increased in a dose dependent manner. The inhibitory effects of AE-COS on the activity and expression level of MMP-2 and MMP-9 related to invasion of cancer cells were examined using gelatin zymography and western blot. In our study, it was found that CPO above 2 μM significantly inhibited on MMP-9 activity as well as MMP-2 activity. Furthermore, CPO reduced the expression of MMP-2 and MMP-9 compared with phorbol-12-myristate-13-acetate (PMA)-stimulated group. The above data provides an evidence that CPO could contribute prevention and treatment of metastasis as a MMP inhibitor.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-98**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Chemical Sporulation and Germination of Mammalian Cells

이준오

국방과학연구소 5본부 3부

Nature finds ways of protecting cellular components and preserving genetic information against external stresses such as nutrient deprivation, desiccation, high temperatures, radiation, and caustic chemicals. For example, bacteria and fungi are covered with a cell wall or robust membrane composed of polysaccharides of peptidoglycans. Certain unicellular organisms, such as diatoms, foraminifera, coccoliths, and rhabdoliths, are encased within exoskeletal shells made of silica or calcium carbonate. However, most mammalian cells do not have a robust membrane or exoskeleton. Instead, they are enclosed in a lipid bilayer, which is fluidic and vulnerable to changes in its environments. Because the surfaces of mammalian cells are not protected or reinforced by a tough coat, it is more difficult to treat mammalian cells in vitro than microbial cells. In this work, three types of mammalian cells were individually coated within metal-polyphenol and silica shells. To maintain the viability of mammalian cells, we performed the whole processes under strictly physiological culture conditions, and carefully selected nontoxic materials, established with toxicity tests.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-99**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Identification of a novel methyl transferase in wobble uridine modification of tRNA

김정욱* 류희정

GIST 화학과

Post-transcriptional modifications of tRNA, especially those located in the anticodon stem loop, enhance the efficiency of translation by modulating codon recognition, translocation, and frameshift. In particular, O-alkylation of wobble uridine is widely conserved among bacteria as 5-oxyacetylation (cmo5U), or 5-methoxylation (mo5U) in Gram-negatives or Gram-positives, respectively. tRNA molecules containing these modifications exhibit expanded codon-degeneracy. Although the biosynthetic pathway of cmo5U has been revealed recently, how mo5U is synthesized still remains unknown. Here, we have identified YrrM, a previously uncharacterized enzyme, is required for the biosynthesis of mo5U in Bacillus subtilis. Also, we have determined the X-ray crystal structure of the protein, bound with a substrate, SAM. Finally, we have analyzed the biochemical properties of the enzyme by determining the oligomerization state in solution, the substrate binding affinity and the in vitro methyl transfer activity. These results collectively support that YrrM is involved in the methylation of the hypomodified ho5U to form mo5U at the wobble position of tRNA in Gram-positive bacteria.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-100**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

TUDCA-incorporated PEG-L-PA thermogel for hepatogenic differentiation of human tonsil derived mesenchymal stem cells

홍자혜 이현정 장서희 정병문*

이화여자대학교 화학나노과학과

Since tauroursodeoxycholic acid (TUDCA) can promote liver regeneration, its influence on tonsil-derived mesenchymal stem cell was investigated. For hepatocyte differentiation, Tonsil-derived mesenchymal stem cell (TMSCs) were seeded into PEG-L-PA thermogel with TUDCA for 3 weeks. The cell-encapsulated 3D matrix was prepared by increasing the temperature of the cell-suspended PEG-L-PA aqueous solution (14.0 wt. %) to 37oC. The gel modulus at 37oC was about 1100 Pa. In TUDCA-incorporated 3D system, TMSCs expressed elevated level of liver specific genes, protein and functions together.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-101**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Multicomponent interactions of type II methanotrophs

이승재* 송민영[1]

전북대학교 화학과 [1]전북대학교 화학과

Methanotrophs consume methane as their sole carbon source and play an essential role in the global carbon cycle by limiting its atmospheric content. These bacteria oxidize methane to methanol using soluble methane monooxygenases having hydroxylase, regulatory, and reductase protein components. Until now, the catalytic mechanism has remained ambiguous due to a lack of atomic-level information about component interactions. We have recently reported the 2.9 Å resolution crystal structure of soluble methane monooxygenase hydroxylase (MMOH) in complex with its regulatory component (MMOB) from Methylococcus capsulatus (Bath). MMOB docks in a canyon formed at the $\alpha_2\beta_2$ interface of the $\alpha_2\beta_2\gamma_2$ MMOH dimer, and its unstructured N-terminus forms a ring-like structure on the MMOH α-subunit. These interactions control O_2, methane, and proton access to the catalytic diiron center at the active site by altering the internal architecture of the α-subunits and effect conformational changes at key active site residues involved in methane oxidation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-102**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization of metabolites in the roots of halophytes

이승재* 정남진[1]

전북대학교 화학과 [1]전북대학교 작물생명과학과

High salinity is a major abiotic stress that effects the growth and development of plants. These stresses can influence flowering, production of crops, defense mechanisms and other physiological processes. Previous studies have attempted to elucidate salt-tolerance mechanisms in order to improve plant growth and productivity in the presence of sodium chloride. One such plant that has been studied in detail is *Salicornia*, a well-known halophyte, which has adapted to grow in the presence of high salt. To further the understanding of how *Salicornia* grows and develops in high saline conditions, *Salicornia herbacea* (*S. herbacea*) was grown under varying saline concentrations (0, 50, 100, 200, 300, 400 mM) and the resulting phenotype, ion levels, and metabolites were investigated. 100 mM NaCl was determined to be the optimal condition for the growth of *S. herbacea* and increased concentration of salts directly diminished the internal concentration of other inorganic ions including Ca^{2+}, K+, and Mg^{2+}ions. Metabolomics were performed on the roots of the plant as a systematic metabolomics study has not yet reported from the roots of *Salicornia*. Using ethylacetate and methanol extraction followed by high resolution ultra-performance liquid chromatography coupled with mass spectrometry (UPLC-MS), 53 metabolites was increased as the concentration of NaCl increase. These metabolites have been linked to stress responses, primarily oxidative stress responses, which increases under saline stress.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.P-103**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Metalloproteins and their functional consequences

이승재* 신기루[1]

전북대학교 화학과 [1]전북대학교 화학과

Zinc finger (ZF) proteins use zinc as a structural co-factor and are often involved in nucleic acid recognition and binding. Although zinc is typically thought to be the physiologically relevant transition-metal ion for ZF protein function, there is evidence that other metal ions, including iron, may replace zinc under certain conditions. Studies focused on the roles of metal coordination and DNA binding for two specific ZF proteins: ST18 (suppression of tumorogenecity 18) and ZIF268 (zinc interacting factor 268) will be presented. ST18 is a non-classical ZF that belongs to the NZF/MyT family of ZFs. It contains six ZF domains, each of which has a Cys$_2$His$_2$Cys motif. The biological function of ST18 is not well understood; however, there is some recent evidence that ST18 regulates inflammation and apoptosis by regulating gene expression of tumor necrosis factor-alpha (TNF-α). We have been studying constructs of ST18 that contain the Cys$_2$His$_2$Cys domains, and have obtained evidence for zinc binding. These studies along with DNA binding studies with the TNF-α promoter will be presented. ZIF268 is a classical zinc finger protein that utilizes a Cys$_2$His$_2$ ligand set to bind zinc and fold into a characteristic $\beta_2\alpha$ structure. The zinc and DNA binding properties of ZIF268 are well understood and it is possible to modify the protein sequence to tune DNA recognition. As part of an effort to understand the role of metal ion identity in function, we performed optical titrations of ZIF268 with ferrous and ferric iron followed by DNA binding studies (monitored by fluorescence anisotropy). We discovered that both ferric and ferrous iron binds to ZIF268, and both forms can bind to target DNA with comparable affinity to Zn-ZIF268; however, the iron bound forms are more susceptible to oxidation than zinc.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.P-104**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Diacetyl atractylodiol inhibits hypoxia-induced angiogenesis by Suppression of Akt-HIF-1α signaling axis

최식원 이광식[1] 서우덕*

농촌진흥청 국립식량과학원 [1]국립식량과학원 작물기초기반과

Hypoxia-inducible factor (HIF)-1α is a key regulator associated with tumorigenesis, angiogenesis, and metastasis. HIF-1α regulation under hypoxia has been highlighted as a promising therapeutic target in angiogenesis-related diseases. Here, we demonstrate that diacetyl atractylodiol (DAA) from Atractylodes japonica (A. japonica) is a potent HIF-1α inhibitor that inhibits the Akt signaling pathway. DAA dose-dependently inhibited hypoxia-induced HIF-1α and downregulated Akt signaling without affecting the stability of HIF-1α protein. Furthermore, DAA prevented hypoxia-mediated angiogenesis based on in vitro tube formation and in vivo chorioallantoic membrane (CAM) assays. Therefore, DAA might be useful for treatment of hypoxia-related tumorigenesis, including angiogenesis

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-105**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Comparative assessment of isoflavones using microwave assisted method, nutritional components and antioxidant properties at growth stage from different parts of soybean [Glycine max (L.) Merrill]

서우덕* 이광식[1] 최식원

농촌진흥청 국립식량과학원 [1]국립식량과학원 작물기초기반과

This work was the first to investigate isoflavones using microwave assisted method and antioxidant effects against DPPH and ABTS from different parts (seeds, leaves, leafstalks, pods, stems, and roots) of soybean plant. The fluctuations of isoflavone, protein, oil, and fatty acid were also conducted to determine in R6• R8 seeds. The R7 seeds exhibited the most predominant isoflavone (1218.1±7.3 μg/g) with the following order: daidzein (48%)>genistein (35%)>glycitein (17%). The second major isoflavone was found in leaves, with 1052.1±10.4 μg/g, followed by R8 seeds>roots>R6 seeds>leafstalks>pods, while stems showed the lowest (57.2±1.7 μg/g). Interestingly, daidzein was observed the highest individual isoflavone with remarkable variations (57.2• 766.8 μg/g), representing approximately 46• 100% of total isoflavone. Protein, oil, and fatty acid exhibited higher contents in R8 than those of R6 and R7 seeds. The antioxidant capacities showed considerable differences, depending upon isoflavone. Our results provide that soybean seeds and leaves may be useful ingredients of functional foods

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

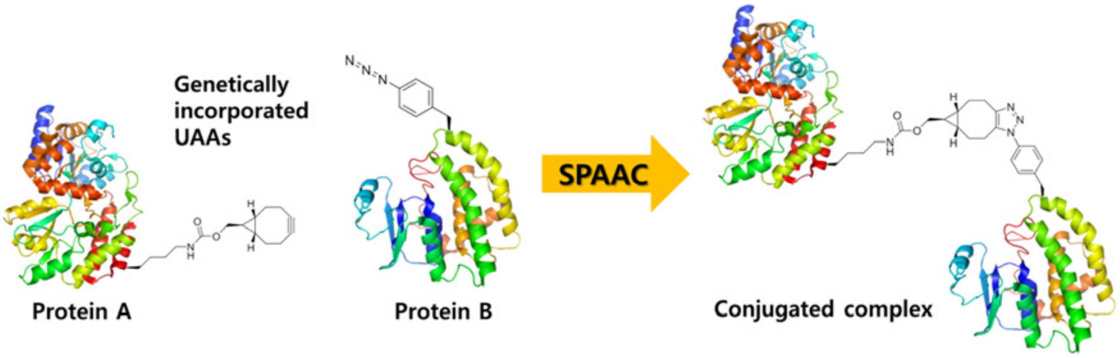
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-106**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Direct protein-protein conjugation by genetically introducing bioorthogonal functional groups into proteins

김상길 이현수*

서강대학교 화학과

Proteins often function as complex structures in conjunction with other proteins. Because these complex structures are essential for sophisticated functions, development of protein-protein conjugates has been of special interest. In this study, site-specific protein-protein conjugation was performed by genetically incorporating an azide-containing amino acid into one protein and a bicyclononyne (BCN)-containing amino acid into the other. Three to four sites in each of the proteins were tested for conjugation efficiency, and three combinations showed excellent conjugation efficiency. The genetic incorporation of unnatural amino acids (UAAs) is technically simple and produces a mutant protein in high yield. In addition, the conjugation reaction can be conducted by simple mixing, and does not require additional reagents or linker molecules. Therefore, this method would be very useful to form protein-protein conjugates and protein complexes of biochemical significance


Genetically incorporated UAAs
Protein A
Protein B
SPAAC
Conjugated complex

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

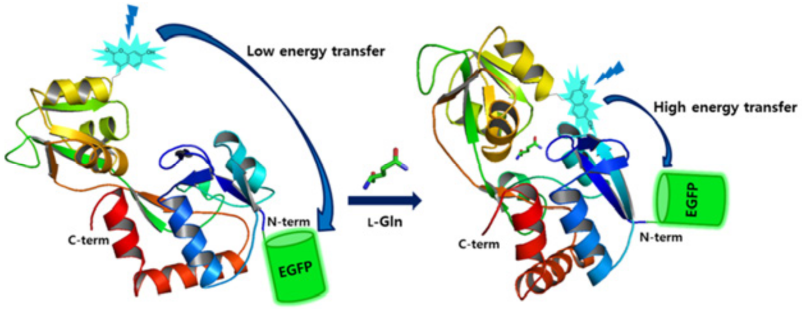
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-107**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Genetically encoded FRET sensors using a fluorescent unnatural amino acid as a FRET donor

이현수* <u>고우석</u>

서강대학교 화학과

FRET sensors based on fluorescent proteins have been powerful tools for probing protein-protein interactions and structural changes within proteins. However, they are intrinsically limited by their large size and the requirement for N- or C-terminal fusions. In this report, a FRET-based sensor was developed by incorporating a fluorescent unnatural amino acid into glutamine-binding protein (GlnBP), which formed a FRET pair with green fluorescent protein (GFP). GFP was fused to the N-terminus of GlnBP, and the fluorescent unnatural amino acid was incorporated into the site for N138 in GlnBP. FRET sensors were tested that contained linkers of different length between GFP and GlnBP, and assay conditions were optimized by changing the pH and salt concentration of the assay buffer. Under optimal conditions, the best sensor protein produced a 1.9-fold increase in the FRET ratio upon L-Gln binding, whereas either no change or minimal change was seen using other amino acids, including the other 19 natural amino acids and D-Gln. This novel design strategy for FRET sensors overcomes the limitations of current FRET sensors, which require the use of two fluorescent proteins. Consequently, our strategy may prove useful for investigating protein-protein interactions and for probing changes in protein conformation.


Low energy transfer
N-term
C-term
EGFP
L-Gln
High energy transfer
C-term
N-term
EGFP

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-108**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Lumazine Synthase Protein Nanoparticle-Gd(III)-DOTA Conjugate as a T1contrast agent for high-field MRI

김한솔 문효진 배윤지 강세병[1,*]

UNIST 생명과학과 [1]UNIST 나노생명화학공학부

With the applications of magnetic resonance imaging (MRI) at higher magnetic fields increasing, there is demand for MRI contrast agents with improved relaxivity at higher magnetic fields. Macromolecule-based contrast agents, such as protein-based ones, are known to yield significantly higher r1 relaxivity at low fields, but tend to lose this merit when used as T1 contrast agents (r1/r2 = 0.5 ~ 1), with their r1 decreasing and r2increasing as magnetic field strength increases. Here, we developed and characterized an in vivo applicable magnetic resonance (MR) positive contrast agent by conjugating Gd(III)-chelating agent complexes to lumazine synthase isolated from Aquifex aeolicus (AaLS). The r1 relaxivity of Gd(III)-DOTA-AaLS-R108C was 16.49 mM−1s−1 and its r1/r2 ratio was 0.52 at the magnetic field strength of 7 T. The results of 3D MR angiography demonstrated the feasibility of vasculature imaging within 2 h of intravenous injection of the agent and a significant reduction in T1 values were observed in the tumor region 7 h post-injection in the SCC-7 flank tumor model. Our findings suggest that Gd(III)-DOTA-AaLS-R108C could serve as a potential theranostic nanoplatform at high magnetic field strength.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-109**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Phosphoprotein phosphatase 1CB (PPP1CB) promotes adipogenesis in 3T3-L1 adipocytes

노경민 강효진* 정상전*

동국대학교 화학과

Obesity has become one of the most common metabolic diseases worldwide. As adipogenesis plays a crucial role in obesity, understanding the molecular networks of adipogenesis is important for identifying medicinal targets of obesity.[1] Although many adipogenesis-controlling transcriptional factors have been proposed, activators that promote the early development of adipocyte are still unknown. Our research demonstrated that phosphoprotein phosphatase 1CB (PPP1CB) plays a crucial role to promote adipocyte differentiation as a potent adipogenic activator. Hormonal stimulation in the early phase of 3T3-L1 adipogenesis in high-fat diet-induced obesity murine models resulted in significant increased expression of PPP1CB. Depletion of PPP1CB dramatically suppressed the differentiation of 3T3-L1 cells into mature adipocytes. Furthermore, knockdown of PPP1CB caused a significant decrease in C/EBPδ expression, which in turn resulted in attenuation of PPARγ, C/EBPα, adiponectin, and aP2. This results of our study demonstrate the functional significance of PPP1CB by linking p38 activation to C/EBPδ expression in early adipogenesis. Finally, our findings suggest that PPP1CB is a promising therapeutic target for the treatment of obesity and obesity-related diseases.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-110**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient Method of Detection Bar Genetically Modified Rice (Oryza sativa L.) by the Loop-Mediated Isothermal Amplification

전승훈 **KIM SUE KYUNG** 김진호 문명진[1] 최지영 김민선 김상현 김영관 여동현 장원철*

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Rice (Oryza sativa L.) is one of the central crops in the world and a basic food that provides nutrition for peoples. A genetically modified (GM) crops and its harvest areas are highly increased in world wide. GM rice tolerance to herbicides or resistance to insect can be increase yield and reduce the use of chemicals for crop protection. Among GM related genes, bar gene is able to provide tolerance from glufosinate-ammonium and active herbicide. Along fast developing of GM crops, many peoples were concerned on the risks of GM crops. Several international organizations and countries were strengthening the supervision and labeling of GM products. In order to perform GM labeling, it is essential to develop methods for detecting the GM in products.Recently, various methods including enzyme-linked immunosorbent assay (ELISA), conventional PCR and competitive PCR have been used for detection of GM. These methods require expensive devices, reagent and sufficient time. Loop-mediated isothermal amplification (LAMP) assay is one of the nucleic acids amplification methods. Advantages of LAMP are high sensitivity, low cost and reduce time consuming.In this study, we have detected the bar gene using LAMP, and our results were confirmed by restriction fragment length polymorphism. Our results showed that sensitivity of LAMP methods are higher than PCR methods (detection limits of LAMP and PCR are 10-3 and 10-2 dilution, respectively). In summary, LAMP assay was found to be 10 fold more sensitive than PCR. We suggested that reliability and sensitivity of LAMP assay are better than PCR for bar gene detection.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-111**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Detection of rifampicin-resistant Mycobacterium tuberculosis by allele specific polymerase chain reaction

최지영 **KIM SUE KYUNG** 김진호 문명진[1] 김민선 전승훈 김상현 김영관 여동현 장원철[*]

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Tuberculosis (TB) is one of the highest infectious diseases in worldwide. World Health Organization (WHO) reported that 40,000 Korean populations have infected TB in 2014. In addition, high mortalities of TB infected patients were significantly related with multidrug-resistant (MDR) Mycobacterium tuberculosis strain. First-line anti-TB drugs are isoniazid, rifampicin, ethambutol and pyrazinamide. Of them, the target of rifampin is the RNA polymerase β–subunit, where inhibits the elongation of mRNA. Previously studies that rpoB gene is encoded to the β-subunit of DNA-dependent RNA polymerase. In addition, several studies demonstrated that mutations of 81bp 'hot-spot' region of rpoB gene were associated about 95% rifampin-resistance. However, conventional detection methods for TB drug resistance were time consuming. For example, gold standard test like dug susceptibility test for Mycobacterium tuberculosis strain takes 6-8 weeks. For this reason, rapid and accurate detection methods of TB are needed for efficient treatment of patients. In this study, we have conducted allele-specific PCR (AS-PCR) for detection of drug-resistant related genes mutations (rpoB 526 and 531 codons). Our results indicated that, the methods provide 100% sensitivity and specificity. In addition, we found that frequencies of 526 and 531 codons are 12.77% and 5.32%, respectively. We suggest that AS-PCR is efficient methods for detection of drug resistance mutation of TB patients.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-112**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ferritin Nanocage and Functional Peptides Binding to α-Enolase Relieve Synovial Inflammation in Rheumatoid Arthritis

김가현 강효진 정상전*

동국대학교 화학과

Rheumatoid arthritis (RA) is one of the most prevalent autoimmune diseases, and antigen-presenting cell (Monocyte and macrophage) and autoantibodies are known to be the main causes thereof. Most recent studies indicate that α-Enolase (ENO1) is over expressed on the cell-surface of monocytes and macrophages of RA patients, resulting in synovial inflammation. [1] Certain peptides can control inflammation by binding to ENO1, however, their proteolytic degradation hampers therapeutic application. In this study, clustering of anti-inflammatory peptides was used to improve their therapeutic efficacy towards rheumatoid arthritis. The increased avidity of the peptide clusters may enhance the binding affinity and increase the biological half-life. Ferritin, a protein nanocage composed of 24 identical protein subunits was used to attain ferritin-peptide nanoclusters. To this end, the target peptide was cloned to both the N- and C-termini of the ferritin monomer and expressed in E. coli. Due to the local symmetry of the N- and C-termini of the ferritin monomers on the surface of the self-assembled nanocage, the target peptides are clustered on the nanocage surface. TEM image of the purified ferritin-peptide nanoclusters revealed well-formed ferritin-peptide nanoclusters without any irregular protein aggregates. Currently, the therapeutic effects of the ferritin-peptide nanoclusters are under investigation using animal models. 1.Bae S, Kim H, Lee N, Won C, Kim HR, Hwang YI, Song YW, Kang JS, Lee WJ: Journal of immunology (Baltimore, Md : 1950) 2012, 189(1):365-372.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-113**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Evaluation and Characterization of Soyasaponins from Germinated Soy Germ

이광식 최식원[1] 서우덕[1,*]

국립식량과학원 작물기초기반과 [1]농촌진흥청 국립식량과학원

Soy germ contains a relatively higher content of bioactive compounds, such as isoflavones, soyasaponins and tocopherols, than the cotyledon. Germinated soy germ (GSG) is a potential enrichment source of bioactive and nutritional components for healthy food products. Soyasaponins have been reported to possess a wide range of benefits, including anti-inflammation, anti-virus, and antioxidant activities, as well as hepatoprotective and cardiovascular protective effects. Separated soy germ was germinated at room temperature for 24hr under water. And then, the extracts and chemical compounds isolated and characterized of soyasaponins from GSG using LC-DAD-CAD and LC-QTOF-Ms/Ms. The soyasaponin contents of GSG showed an increase of 1.6 times during 24hr germination. The isolated compounds were soyasaponins in GSG and they were identified as soyasaponin Ab. Soyasaponin Ab constituted more than 80% of soyasaponins contents in GSG extracts. Consequently, our results suggest that GSG may be utilized as an effective anti-inflammtory health food, additives in human and feed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-114**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Genetic variant in SORL1 is associated with Alzheimer's disease in Asian population: A Replication Study and Meta-Analysis

김민선 **KIM SUE KYUNG** 김진호 문명진[1] 최지영 전승훈 김상현 김영관 여동현 장원철[*]

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

In two large genome-wide associated studies (GWAS) demonstrated that Sortilin-related receptor (SORL1) was associated with late-onset AD in several populations. SORLA protein encoded by SORL1 gene is the member of low-density lipoprotein receptor family that binds lipoproteins including ApoE-containing particles. For this reason, many previous studies have investigated the association between SORL1 polymorphisms and risk of AD in various ethnicities. However, results of the relationship between SORL1 polymorphisms and risk of AD were inconsistent between individual studies.In this study, we have performed case-control study of the association between rs12285364 polymorphism of SORL1 and risk of AD in Korean population. In addition, we have re-evaluated the association between rs12285364 polymorphism and risk of AD in Asian population using meta-analysis. Our results showed that rs12285364 polymorphism was statistically not associated with risk of AD in Korean population [OR = 1.170 (95% CI: 0.622-2.204); p = 0.626]. In contrast, we found that rs12285364 polymorphism was significantly associated with increased risk of AD in Asian population [heterozygote model: OR = 1.29 (95% CI = 1.05-1.58); dominant model: OR = 1.30 (95% CI = 1.06-1.58)].In summary, our results demonstrated that rs12285364 polymorphism was significantly associated with risk of AD in Asian population whereas this polymorphism was not associated with Korean AD. However we should need a validation of the meta-analysis using various case-control studies with larger sample size to confirm these conclusions.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-115**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Detection of BER enzymes by real-time PCR using PNA probes

김은택 홍인석*

공주대학교 화학과

It is important to detect the DNA repair enzymes to understand the role of their activity in our body. hOGG1 is an 8-oxoguanine DNA glycosylase which acts both as a N-glycosylase and an AP-lyase. The N-glycosylase activity releases damaged purines from double stranded DNA, generating an apurinic (AP) site. The AP-lyase activity cleaves 3′ to the AP site leaving a 5′ phosphate and a 3′-phospho-α, β-unsaturated aldehyde. UDG is catalyses the release of free uracil from uracil-containing DNA. UDG efficiently hydrolyzes uracil from single-stranded or double-stranded DNA.We study detection of hOGG1 and UDG by real-time PCR using PNA probes. We designed the specific single strand DNA (8-oxodG ssDNA, uracil ssDNA), which has a 8-oxoguanine and uracil nucleotide (located at the center of sequence) and primer annealing sequences (located at the each terminal sites of sequence). Also, we designed the short complementary PNA probes, which has fluorophore and quencher. PNA probes, each complementary to hOGG1 and UDG ssDNA, has diffirence fluorophore. After addition of short complementary ssDNA to the 8-oxodG/uracil ssDNA solution, the aliquot of enzymes was added to the dsDNA. In the presence of enzymes, the target DNA was cleaved to the short oligomer, which can not be efficiently amplified by real-time PCR. Consequently, we can monitored the Ct values of amplified DNA using PNA probes,

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-116**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Recombinant Secondary Antibody Mimic as a Target-specific Signal Amplifier and an Antibody Immobilizer in Immunoassays

최봉서 최혁준 강세병*

UNIST 생명과학부

We construct a novel recombinant secondary antibody mimic, GST-ABD, which can bind to the Fc regions of target-bound primary antibodies and acquire multiple HRPs simultaneously. We produce it in tenth of mg quantities with a bacterial overexpression system and simple purification procedures, significantly reducing the manufacturing cost and time without the use of animals. GST-ABD is effectively conjugated with 3 HRPs per molecule on an average and selectively bind to the Fc region of primary antibodies derived from three different species (mouse, rabbit, and rat). HRP-conjugated GST-ABD (HRP-GST-ABD) is successfully used as an alternative to secondary antibodies to amplify target-specific signals in both ELISA and immunohistochemistry regardless of the target molecules and origin of primary antibodies used. GST-ABD also successfully serves as an anchoring adaptor on the surface of GSH-coated plates for immobilizing antigen-capturing antibodies in an orientation-controlled manner for sandwich-type indirect ELISA through simple molecular recognition without any complicated chemical modification.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-117**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Peptide microarrays for screening of apoptosis inducing Pre-miRNA-155 binding peptides

현지영 신인재*

연세대학교 화학과

MicroRNAs (miRNAs), short single-stranded noncoding RNAs of ~22 nucleotides, regulate expression of target genes through either degradation of target mRNAs or inhibition of protein translation. These RNAs play crucial roles in a wide range of physiological processes, including development, cell proliferation and differentiation and apoptosis. MicroRNA-155, one of the most potent miRNAs that suppress apoptosis in human cancer, is overexpressed in numerous cancers and it displays oncogenic activity. Peptide microarrays, constructed by immobilizing 185 peptides containing the C-terminal hydrazide onto epoxide-derivatized glass slides, were employed to evaluate peptide binding properties of pre-miRNA-155 and to identify its binding peptides. Two peptides, which were identified based on the results of peptide microarray and in vitro Dicer inhibition studies, were found to inhibit generation of mature miRNA-155 catalyzed by Dicer and to enhance expression of miRNA-155 target genes in cells. In addition, the results of cell experiments indicate that peptide inhibitors promote apoptotic cell death via a caspase-dependent pathway. Finally, observations made in NMR and molecular modeling studies suggest that a peptide inhibitor preferentially binds to the upper bulge and apical stem-loop region of pre-miRNA-155, thereby suppressing Dicer-mediated miRNA-155 processing.

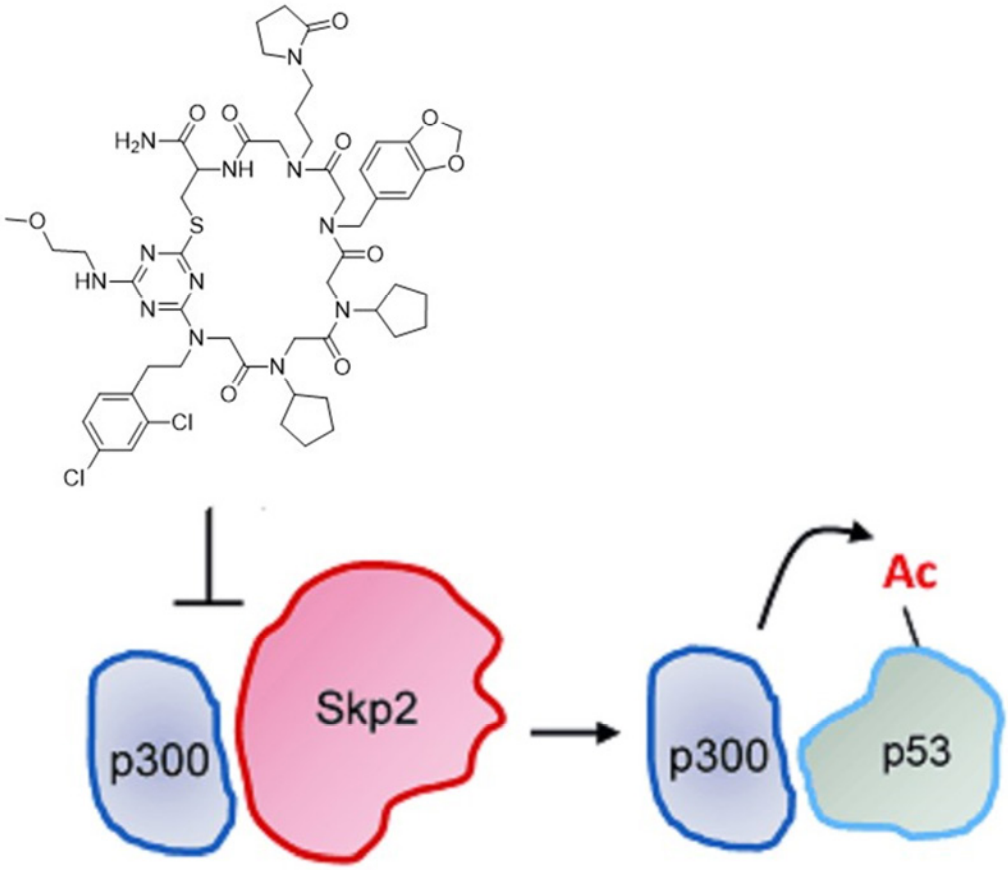
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-118**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Identification of a Chemical Inhibitor of the Skp2/p300 Interaction

현유정 임현석*

POSTECH 화학과

Skp2 is thought to have two critical roles in tumorigenesis. As part of the SCFSkp2 ubiquitin ligase, Skp2 drives the cell cycle by mediating the degradation of cell cycle proteins. Besides the proteolytic activity, Skp2 also blocks p53-mediated apoptosis by outcompeting p53 for binding p300. Herein, we exploit the Skp2/p300 interaction as a new target for Skp2 inhibition. An affinity-based high-throughput screen of a combinatorial cyclic peptoid3 library identified an inhibitor that binds to Skp2 and interferes with the Skp2/p300 interaction. We show that antagonism of the Skp2/p300 interaction by the inhibitor leads to p300-mediated p53 acetylation, resulting in p53-mediated apoptosis in cancer cells, without affecting Skp2 proteolytic activity. Our results suggest that inhibition of the Skp2/p300 interaction has a great potential as a new anticancer strategy, and our Skp2 inhibitor can be developed as a chemical probe to delineate Skp2 nonproteolytic function in tumorigenesis.


p300
Skp2
p300
p53
Ac

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-119**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Decreased level of glutathione in endoplasmic reticulum by ER stress

강철훈

경희대학교 동서의학대학원

The redox balance in endoplasmic reticulum (ER) may play important roles in human diseases since its imbalance may interfere disulfide bond formation of the newly synthesized proteins in the ER, which may result in accumulation of unfolded proteins, the ER stress. The balance is contributed by the glutathione (GSH). Hence, in this study, using an ER GSH-selective fluorescent probe and confocal microscopy, whether the ER stresses may induce alteration of GSH levels or not was pursued. It was found that it shows that the ER stresses such as brefeldin A- and tunicamycin-treatments induced decrease in GSH level in ER.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-120**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Discovery of a small-molecule inhibitor of protein–microRNA interaction using binding assay with a site-specifically labeled Lin28

임동현 박승범[1,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

MicroRNAs (miRNAs) regulate gene expression by targeting protein-coding transcripts that are involved in various cellular processes. Therefore, miRNA biogenesis has been recognized as a novel therapeutic target. Especially, the let-7 miRNA family is well known for its tumor suppressor functions and is downregulated in many cancer cells. Lin28 protein binds to let-7 miRNA precursors to inhibit their maturation. Herein, we developed a FRET-based, high-throughput screening system to identify small-molecule inhibitors of the Lin28–let-7 interaction. We employed unnatural amino acid mutagenesis and bioorthogonal chemistry for the site-specific fluorescent labeling of Lin28, which ensures the robustness and reliability of the FRET-based protein–miRNA binding assay. Using this direct binding assay, we identified an inhibitor of the oncogenic Lin28–let-7 interaction. The inhibitor enhanced the production of let-7 miRNAs in Lin28-expressing cancer cells and reduced the level of let-7 target oncogene products.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-121**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Label-free quantitative proteome profiling of cerebrospinal fluid for prognosis of stem cell therapy of stroke by using a rat model

고승익 이상원*

고려대학교 화학과

Stem cell therapy offers promising therapeutic effect for ischemic damage in stroke by regenerating damaged neural cells. The most promising stem cells about stem cell therapy are Human adipose-derived stem cells (hASCs). The hASCs are capable of performing immunomodulation and regeneration after injury, and promoting angiogenesis and neurogenesis. For these reasons, hASCs have been investigated as a promising stem cell candidate for treatment of strokes. Cerebrospinal fluid (CSF) can reflect the pathophysiology of various neurological disorders that occur to the central nervous system (CNS) as CSF involves in physiological control of a brain to maintain a stable CNS condition. The quantitative analysis of CSF proteome change after stem cell transplantation in the stroke animals can potentially reveal the effect of stem cells on host CNS of a stroke rat model after stem cell treatment. In this study, we investigated secretome function of hASCs conditioned media in order to reveal hASCs secreted proteins function which expected to show a therapeutic effect intravenous injection. Then, we obtained CSF samples from a rat model of stroke which is subjected to intravenous injection of hASCs 9 days earlier as well as the control CSF samples with using LC-MS/MS data on the tryptic peptide samples of CSF samples, proteome changes in cerebrospinal fluid (CSF) after the injection of hASCs were analyzed by using label-free quantitative proteomics. In summary, we identified 2,928 protein groups of 18,008 non-redundant peptides and 102 differentially expressed proteins (DEPs, >2.0 fold & p-value < 0.1). In further study, signaling pathways will be analyzed from DEPs in order to identify the proteins responsible for hASCs induced neuroregenararation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-122**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Metabolomics analysis of Nuruk starters for Korean traditional wine, Makgeolli, with different temperatures during fermentation

김범태* <u>이상화</u>[1] 송정섭[2]

전북대학교 큰사람교육개발원, 생리활성물질연구소 [1]전북대학교 생리활성소재과학과 [2]전북대학교 화학과

Nuruk starter is one of the crucial ingredients for brewing of Korean traditional wine, Makgeolli. During fermentation of Nuruk, continuous variation of diverse microbes in species and their prosperties has occurred and thereby their corresponding metabolite variation is accompanied with them, which eventually make crucial contribution to brewing process and the quality of final brew. While in our previous work, the primary metabolic variation of Nuruk starters with different raw materials and water content was investigated in time-dependent manner during fermentation, in the present work, metabolomics analysis of Nuruk starters with different temperatures during fermentation was investigated. The raw materials (mass ratio) used in preparation of Nuruk disks was barley and green gram (3.3:0.52, w/w) and the initial water content was 26%. The Nuruk disks were incubated at two different temperatures, 30 and 40 oC for 30 days under 70% of humidity which was reduced to 50% after 4th day. The Nuruk samples were named as TN-E and F, and collected from three parts from disk, i.e. whole, inner, and surface part of disk, at 0, 3rd, 6th, 10th, 20th, 30th day after start of fermentation. All samples were chemically modified via oximation and subsequent in-situ silylation, and analyzed with GC-MS for the analysis of variation of primary metabolites including sugars and sugar alcohols, amino acids, several organic acids and fatty acids. The general features are that the metabolites observed in each Nuruk starters were same in their kinds irrespective of temperature, but showed different patterns in their amounts in each metabolite-dependent and time-dependent manner. The notable observation was that the amounts of metabolites in whole and inner part incubated at 30oC are relatively much than those at 40oC, which suggesting that the favorable environment is unlikely to be constituted for growth of diverse microorganisms at relativlely higher temperature. The most types of metabolites are included, i.e.

phosphoric acid, succinic acid, malic acid, xylose, fructose, galactose, xylitol, mannitol, palmitic acid, linoleic acid, and oleic acid. However, in surface part, this patter is not observed obviously. The other observation deserved to mention is that the amount variation patterns of some metabolites of whole and inner part are exhibited in the fermentation stage dependent manner. The amount of most monosugar metabolites including xylose, fructose, galactose, glucose, and lactose decreased rapidly at the early stage (0-3 day) and whereafter maintained invariable. In contrast, the amount increases steadily at the early stage (0-10 day) and after that time decrease slowly for the metabolites such as phosphoric acid, succinic acid, oleic acid, xylitol, and glycerol (in whole), and palmitic acid, linoleic acid, and oleic acid (in inner part). These observations would be associated with the growth and transition of diverse microorganisms over fermentation time. The information on metabolic variation of Nuruk fermentation would be useful to make better reference point of quality levels of Nuruk starters. (This work was carried out with the support of the “Cooperative Research Program for Agricultural Science & Technology Development (Project No. PJ009998022016)”, Rural Development Administration, Republic of Korea.)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-123**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Discovery of an mTORC1 regulating compound, having a novel mode-of-action, LRS-RagD interaction modulation

정진주 김종훈[1] 조완상[2] 박승범[2,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학과 [2]서울대학교 화학부

Mechanistic target of rapamycin complex 1 (mTORC1) regulates many fundamental features of cell growth and proliferation in response to growth factor, nutrient, stress signal and amino acids. Owing to its central role of mTORC1 in cellular system, it is no wonder that mTORC1 signaling is deregulated in various disease model and considered as a potential therapeutic target. Recently, Ras-like GTPase (Rag) has reported as a major component to activate mTORC1 in an amino-acid dependent manner, and leucyl-tRNA synthetase (LRS) charging leucine to a cognate tRNA have reported as an interaction partner of the RagD protein as a leucine sensor and a GTPase activating protein for RagD, and finally induced activation of mTORC1.To modulate mTORC1, the amino-acid dependent mTORC1 activation is quite less familiar than targeting mTORC1 itself or PI3K-Akt signaling pathway for mTORC1 activity modulation. However, we hypothesized that modulation of LRS-RagD interaction could be a novel and effective strategy in the way that it is a nutrient dependent signaling pathway and targeting specific protein-protein interaction (PPI).To identify mTORC1 regulating compounds having LRS-RagD interaction modulation, we conducted ELISA-based high-throughput screening (HTS) of leucyl-tRNA synthetase (LRS)–Ras-related GTP-binding protein D (RagD) interaction. This screening exercise led to the identification of an effective hit compound, 21f, which regulated the amino acid-dependent activation of mechanistic target of rapamycin complex 1 (mTORC1) activity via specific inhibition of LRS–RagD interaction. 21f could serve as a research tool with a novel mode of action for specific modulation of mTORC1 signaling pathway.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-124**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Detection of Helicobacter pylori with Dual-Modal Fluorescent Magnetic Glyconanoparticles

현지영 신인재*

연세대학교 화학과

H. pyroli, which colonizes the human stomach, is one of the most widespread infectious pathogens affecting nearly one-third of the world's population. H. pyroli causes chronic gastritis, which may lead to peptic ulcer disease and gastric cancer. Therefore, sensitive detection of H. pylori is crucial for diagnosis and treatment of H. pylori associated diseases. The cell surface of this pathogen frequently contains adhesins that recognize specific host cell glycans, as exemplified by the well-characterized blood group antigen-binding adhesin (BabA). In this case, infection of hosts by H. pyroli is triggered by binding of BabA to Leb present in the gastric mucosa. Owing to their unique roles, H. pylori adhesins have been actively investigated. In the present study, to detect H. pyroli expressing BabA, we prepared dual-modal fluorescent magnetic glyconanoparticles by conjugating aminoethylated Lea, Leb and H1 oligosaccharides to carboxy-containing fluorescent magnetic nanoparticles. The successful preparation of glyconanoparticles was examined by using zeta potential and transmission electron microscopy (TEM). Fluorescence microscopy analysis shows that H1- and Leb-conjugated nanoparticles but not Lea-conjugated nanoparticles bind to BabA displaying H. pylori. In addition, glyconanoparticles block adhesion of H. pylori to mammalian cells, suggesting that they can serve as inhibitors of infection of host cells by this pathogen. It has been also shown that owing to their magnetic properties, glyconanoparticles are useful to enrich adhesin expressing H. pylori. The combined results indicate that dual-modal glyconanoparticles are biocompatible and that they can be employed to sensitively detect pathogens including H. pylori.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-125**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Aptamosomes as dual-drug delivery system for the treatment of MCF-7 breast cancer cells and breast cancer stem cells

김동민 김동은*

건국대학교 생명공학과

Recent studies had demonstrated that metformin and aspirin (sodium salicylate) has surprisingly a potential for anti-cancer effect by inhibiting AMPK-mTOR signaling pathways. Therefore, the purpose of this study was to determine whether aptamer-conjugated liposomes co-encapsulating metformin and sodium salicylate could enhance the anti-cancer efficacy on breast cancer cells and breast cancer stem cells. We designed a drug-encapsulating liposome conjugated with two DNA aptamers specific to the transmembrane glycoprotein mucin 1 antigen (MUC1) and cell surface glycoprotein CD44 antigen (CD44) respectively. MUC1 is known as tumor surface marker significantly expressed on various epithelial cancer cells such as breast cancer and CD44 is recognized as a marker for cancer stem cells. The MUC1 aptamer conjugated liposome, called aptamosome was prepared according to the previously published PSMA-aptamosomes method with slight modification. We have explored a novel strategy of delivering dual-drug specifically to the MCF7 breast cancer cells by using MUC1-aptamosomes. Similar to the MUC1 monoclonal antibody, MUC1-aptamosomes showed intense cell specific binding fluorescence signals to MCF7 breast cancer cells. We then examined the cytotoxicity of dual-drug-encapsulating MUC1-aptamosomes to MCF7 cells. We also demonstrated that dual-drug-encapsulating liposomes are significantly more cytotoxic than only dual-drug treatment. We suggest that the encapsulation of drugs with aptamer conjugated liposomes can be a useful drug delivery system for treatment of breast cancer.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-126**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Drug discovery for the development of Tauopathies therapeutics by HCS/HTS of pDOS library

신영희 박승범*

서울대학교 화학부

Neurofibrillary tangle (NFT) is mainly composed of hyperphosphorylated tau proteins and is the pathological hallmark of Alzheimer's disease along with extracellular amyloid beta plaque. NFTs are also found in Parkinson's disease, Frontotemporal dementia, Chronic traumatic encephalopathy, Progressive supranuclear palsy, etc. and theses diseases are collectively called tauopathies. In order to discover novel compounds that can interrupt abnormal tau aggregation, we focused on hyperphosphorylation and assembly of abnormal tau as phenotypes for the high content screening of pDOS (privileged-substructure based diversity oriented synthesis) compounds. The selected effective compound was further carefully modified by conjugating UV-activated linker and click handle to use as the target identification (FITGE) probe. Potential target proteins are validated by biochemical and biophysical analyses.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.P-127**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Cell Penetrate Peptide-Gemcitabine Conjugates for Enhancing Drug Delivery Efficiency against Cancer Cells

김유민 이연*

서울대학교 화학부

Pancreatic cancer is one of the most fetal cancer and has a narrow chemotherapy. The current chemotherapy of pancreatic cancer is a gemcitabine.Gemcitabine is a deoxycytidine analogue with two fluorine atoms that inhibits the DNA replication of cancers and it registered as an anticancer drug for the treatment of a number of different solid tumors including non-small cell lung (NSCL), pancreatic and many other type of cancer. However, gemcitabine is a polar drug with low membrane permeability, so it requires high drug does that causes drug resistance. The resistance especially, deficiency of equilibrative nucleoside transporters (hENT1s) that transfer the gemcitabine from extracellular to intracellular state, hinder gemcitabine from translocating across cell membrane. And high dose of gemcitabine that is required to translocate cell membrane leads to serious side effects.Herein, we designed cell penetrating peptide (CPP)-gemcitabine conjugates for intracellular delivery efficiently. The main feature of CPPs is that they are able to penetrate the cell membrane at low concentrations through endocytosis and direct translocation. The CPP-gemcitabine conjugates are composed of a disulfide linker cleavable by glutathiones that are relatively abundant in cancer cells. CPP-gemcitabine conjugates can penetrate the cell membrane at lower concentration than gemcitabine. This reduces side effects of anticancer drugs and increases efficiency. We anticipate that the pathway of cellular uptake of CPP-gemcitabine conjugates without using chiral receptors and transporters will be good treatment for the resistant cancer cells.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-128**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Cancer cell selective chemotherapeutic and imaging method : dual-targeting delivery system

박수길 신인재*

연세대학교 화학과

Although many anticancer agents have developed to treat cancer, these show many unwanted normal cell death because of deficiency of selectivity on cancer cell. Additionally, tumor imaging agents also exhibit low target-to-background ratios. The elegant methods that more specifically target cancer cells need to be developed for the improvement of chemotherapeutic efficacy and diagnosis. Here we designed, synthesized and explored the effectiveness of a dual-targeting delivery system that targets cancer cells more selectively, in an effort aimed at improving the tumor selectivity of therapeutic and imaging agents. The new delivery system is composed of a synthetic ligand (octreotide) of somatostatin receptors, a dipeptide substrate for cathepsin B, and a fluorophore or an anticancer agent. The fluorophore-conjugated delivery system was found to be applicable for specific fluorescence imaging of cancer cells that express both somatostatin receptors and cathepsin B. In addition, the anticancer agent containing delivery system leads to the death of cancer cells specifically. In contrast to cancer cells, normal cells that do not produce both somatostatin receptors and cathepsin B at high levels are unaffected by the delivery system. The new dual-targeting approach has the capability of overcoming obstacles associated with current chemotherapeutic and imaging methods.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-129**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enhancing perhydrolase activity of *Candida antarctica* lipase B by modification of the potential water channel residue

전민정 박성순* 정수현*

성신여자대학교 화학과

Lipases are widely used biocatalysts in preparation of enantiopure chiral secondary alcohols through kinetic resolutions. Especially, lipase B from *Candida antarctica* (CAL-B) is one of the most widely used catalysts because of high regio-, chemo-, enantioselectivity. Also, CAL-B has already been studied in enzyme field. In addition, perhydrolase activity of CAL-B was identified. The CAL-B is able to produce epoxides from carboxylic acids and alkenes with hydrogen peroxide as an oxidant. In this study, we would like to report enhancing perhydrolase activity of CAL-B through modification near the potential water channel.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-130**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Redesign of *Candida antartica* lipase B for enhancing enantioselectivity towards Tetrahydrofuran-2-carboxylate

김영현 박성순[1,*] 정수현[1,*]

성신여자대학교 생명과학화학부 [1]성신여자대학교 화학과

Enzyme-catalyzed kinetic resolution is one of the strongest tools in preparation of both enantiomers. Although lipase-catalyzed kinetic resolution is widely used in preparation of many optically pure chiral alcohols, lipase-catalyzed kinetic resolution towards chiral acids is challengeable. The acyl binding pocket of lipase is too large to distinguish each enantiomer of tetrahydrofuran-2-carboxylate. Enantiopure tetrahydrofuran-2-carboxylate (THFC) is particularly important in the province of pharmacy, as chiral building blocks in preparation of bioactive compounds. *Candida antarctica* lipase B (CAL-B) shows low enantioselectivity towards hydrolysis of methyl tetrahydrofuran-2-carboxylate. In this study, we altered the residues near the active site to construct a hydrogen bond or repulsive interaction with the oxygen atom of THFC. Several mutants showed not only higher enantioselectivity but also reverse enantio-preference compared to the wild-type enzyme.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-131**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Isolation of the single-stranded DNA aptamers specifically binding Nucleocapsid protein of Severe Acute Respiratory Syndrome Coronavirus

이태균 정용주*

국민대학교 생명나노화학과

Nucleocapsid protein (N) of Severe Acute Respiratory Syndrome coronavirus (SARS-CoV) is considered as a potential target of the vaccine development of SARS. Through a Systematic Evolution of Ligand by Exponential enrichment (SELEX), the single-stranded DNA (ssDNA) aptamers bound to the N protein were selected from ssDNA library which randomly consists of 40 nucleotide sequences. In 11th round of SELEX, some ssDNA aptamer candidates were isolated, especially candidate 3, 4, 7, 8, and 9 were more specific bound to the N protein than others. For competitive ELISA, the inhibition of the prime aptamer candidates was increased as the aptamer concentration increased. These aptamers are looking forward to developing potential molecular probes for diagnosis and therapy for SARS.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-132**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Detection of exon 19 deletion in EGFR gene using quencher-free fluorescent DNA and graphene oxide

서지나 김동은*

건국대학교 생명공학과

Mutations in epidermal growth factor receptor (EGFR) have been known as prediction index that can be used to monitor the tumor response against drugs such as tyrosine kinase inhibitors in NSCLC. About 50 % of NSCLC patients possess deletion of several sequences in exon 19 of EGFR gene. As less invasive method for detection of EGFR exon 19 deletion mutation is required, we developed a simple PCR-based detection of EGFR exon 19 deletion gene in plasma of NSCLC patients by using quencher-free fluorescent probe DNA and graphene oxide (GO). In the presence of the exon 19 deletion mutation, which is fully complementary to the probe DNA, the probe anneals to the junction sequence (mutant type). The fully annealed DNA probe was then degraded by the 5′ to 3′ exonuclease activity of *Taq* DNA polymerase during PCR, releasing the fluorophore from the probe DNA. In contrast, wild type of exon 19 gene would allow the probe DNA to be annealed partially to the template DNA. The partially annealed probe DNA would be digested by *Taq* polymerase, releasing a fragment of probe DNA. When GO was added to each reaction solution, it produced different fluorescence signals; enhanced fluorescence was observed due to the released fluorophore from the probe DNA that was not adsorbed onto GO, whereas fluorescence was quenched with fragmented single stranded probe DNA that was easily adsorbed onto GO. The fluorescence signal caused by the exon 19 deletion mutation gene was also quantitatively correlated with amount of the mutant gene. Thus, we believe that the GO-based fluorometric assay can be applicable for diagnostic detection of the exon 19 deletion in EGFR gene.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-133**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Discovery of novel chemical compounds that inhibit the activities of SARS coronavirus helicase

표소희 정용주*

국민대학교 생명나노화학과

Severe acute respiratory syndrome (SARS) coronavirus helicase/NTPase is an essential protein for virus replication and regarded as an attractive target for antiviral therapy. In this study, we report two novel compounds, 7-ethyl-8-mercapto-3-methyl-3,7-dihydro-1H-purine-2,6-dione (EMMDPD) and N-(4-((4,6-dioxo-2-thioxotetrahydropyrimidin-5(2H)-ylidene)methyl)phenyl)acetamide (DTPMPA), potently inhibit the SARS coronavirus helicase in vitro by affecting the ATPase activity as well as the dsDNA unwinding activity. We measured the % inhibition by increasing the concentration of the compounds, and IC50 values were determined. We also observed that the compound did not show cytotoxicity up to 80 μM concentration. Our results suggest that the compounds might serve as SARS coronavirus inhibitor.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-134**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Improvement of PCR specificity and efficiency with polyethylene glycol-engrafted nano-sized graphene oxide

김효령 김동은*

건국대학교 생명공학과

Polymerase chain reaction (PCR), a versatile DNA amplification method, is a fundamental technology in modern life sciences and molecular diagnostics. After multiple rounds of PCR, however, nonspecific DNA fragments are often produced and amplification efficiency and fidelity decrease. Here, we demonstrated that polyethylene glycol-engrafted nano-sized graphene oxide (PEG-nGO) can significantly improve PCR specificity and efficiency. PEG-nGO allows specificity to be maintained even after multiple rounds of PCR, allowing reliable amplification at low annealing temperatures. PEG-nGO decreases nonspecific annealing of single-stranded DNA (ssDNA), such as primer dimerization and false priming, by adsorbing excess primers. Moreover, PEG-nGO interrupts reannealing of denatured template DNA by preferentially binding to ssDNA. Thus, PEG-nGO enhances PCR specificity by preferentially binding to ssDNA without inhibiting DNA polymerase, which is analogous to the role of single-stranded DNA binding proteins.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-135**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fluorescent detection of mutant genomic DNA harboring point mutation using Rolling Circle Amplification and Graphene Oxide

구남인 김동은*

건국대학교 생명공학과

The T790M point mutation of epidermal growth factor receptor (EGFR) is one of major cause of resistance to tyrosine kinase inhibitor drugs, such as Gefitinib. In this study, we adopted rolling circle amplification (RCA) and graphene oxide (GO) to detect T790M mutation in genomic DNA extracted from lung cancer cells. RCA is an isothermal DNA amplification method that uses circular DNA template. We have selectively amplified the target gene containing T790M point mutation using selective ligation of the padlock template DNA and subsequent RCA procedure. In the absence of the target mutant gene, gDNA was not amplified as compared with the mutant gene due to absence of ligated padlock template. The single-stranded RCA product containing the T790M point mutation was annealed with the fluorescent PNA probe. The probe PNA was not adsorbed onto GO with unquenched fluorescence. However, in the absence of the target gene amplification by RCA, the fluorescent probe PNA was readily adsorbed onto GO and its fluoresence was quenched. Thus, specific detection of the point mutation was feasible by RCA procedure combined with GO-based fluorescence detection platform.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-136**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of a new inhibitor against a highly conserved bacterial protease

박효진 김석희*

서울대학교 화학부

Protein quality control, refolding or removal of misfolded proteins, is essential for cellular life. DegP/HtrA, a 48-kDa serine protease, is a major protease in Escherichia coli for periplasmic protein quality control, and is implicated in various stress-response pathways. Since DegP/HtrA proteases are highly conserved and are implicated in the virulence of many pathogenic bacteria, they are potential targets for the development of a novel class of antibiotics. Recently, a variant of DegP, DegPR207P/Y444A was reported to have a lethal effect to E.coli and this lethality was suppressed by an extragenic suppressor, a variant form of an outer membrane lipoprotein, Lpp+Leu. In the present study, 10 more potent inhibitors against DegP were picked out of Lpp variant library with screening method we developed. Subsequently, the inhibition effect was confirmed with various methods in vivo and in vitro. From these results, we expect to establish the inhibition mechanism of Lpps against DegP, contributing to the development of small molecular inhibitors.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-137**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Label-Free Target Identification Using In-Gel Fluorescence Difference via Thermal Stability Shift

하재영 박승범[1,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

Target engagement is a prerequisite for therapeutic effects of bioactive small molecules, so unbiased identification of their target proteins can facilitate drug discovery and chemical biology research. Structural modifications of bioactive natural products for target identification have accompanied potential problems such as synthetic difficulty, limited supplies from natural sources, and loss of original efficacy. Herein, we developed a label-free method for proteome-wide target identification using in-gel fluorescence difference caused by thermal stability shift, namely TS-FITGE. Quantitative intra-gel image analysis of each protein spot led to target proteins with shifted thermal stability upon drug engagement, and plotting of melting curves by inter-gel analysis confirmed the positive targets. We demonstrated the robustness and applicability of TS-FITGE method by identifying target proteins, including membrane-bound proteins, of bioactive complex natural products. Furthermore, we identified and functionally validated nucleophosmin as a novel target protein of hordenine, a natural product upregulator of in vitro translation.

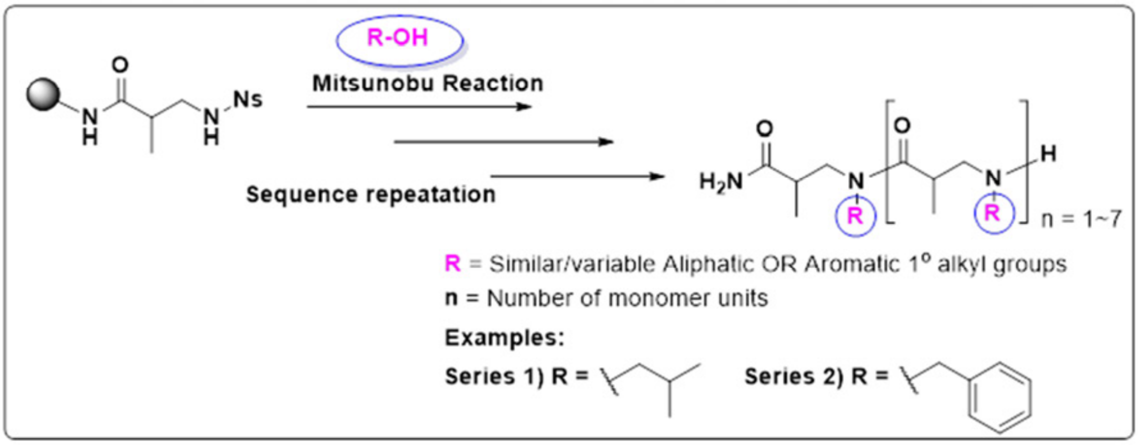
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-138**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

An Expedient Solid-Phase Method for Synthesis of Diversely N-Substituted Oligomers of β2-Homoalanines

Ganesh Sable 임현석*

POSTECH 화학과

The functionalized β-peptoid foldamers have potential applicability in biomedical research. Well-defined positioning of amino acid side chain functionalities in three dimensions is important to acquire and exhibit foldameric properties. Recently, we introduced a new class of peptoid foldamers with backbone chirality, called α-ABpeptoids, which are composed of oligomers of N-substituted β2-homoalanines. Gratifyingly, these oligomers displayed a characteristic CD spectral feature resembling of polyproline type II (PPII) helices, suggesting that they adopt ordered folding conformations. Here, we introduce an efficient solid-phase synthesis protocol to incorporate diverse N-substitutions at N-side chains of β2-homoalanines peptoids up to 8 residues in length. A standard Mitsunobu reaction was applied for these N-substitutions using aliphatic (isobutyl) or aromatic (benzyl) primary alcohols. Furthermore, CD spectroscopic investigations of these series of β2-peptiods with length, temperature and solvent dependency are underway. Moreover, this solid-phase synthetic protocol can serve as an effective method to build a library of β2-peptoids with variable N-substitutions on N-side chain which may lead to develop new functional materials.


R-OH
Mitsunobu Reaction
Sequence repeatation
O
N
H
N
H
Ns
H$_2$N
N
R
H
n = 1~7
R = Similar/variable Aliphatic OR Aromatic 1^o alkyl groups
n = Number of monomer units
Examples:
Series 1) R =
Series 2) R =

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-139**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Construction of a Vast One-Bead One-Compound Library of Cyclic Peptoids

신민현 임현석*

POSTECH 화학과

Affinity-based screening with one-bead-one-compound (OBOC) library is a powerful screening technology that enables to rapidly discover a bioactive molecules for target proteins. On-bead screening with OBOC library has several advantages. First, the OBOC library with synthetic organic molecules or peptidomimetics can be easily synthesized using split and mix method. Second, this screening method enables a large number of library molecules to be screened simultaneously by incubating with a target protein in a single test tube. However, current OBOC library generally contains less than 1 million of beads due to the relatively large size of the bead (100 μm, 1.72 x 106 beads/g), so these diversity level of library usually leads hit compounds with moderate binding affinity. In this study, synthetic method for cyclic peptoid library using tiny beads (10 μm, 1.95 x 109 beads/g) was developed to increase diversity of OBOC library. This library has several advantages. First, because the cyclic peptoid is known for resistant to proteases and far more cell permeable than peptide, it can be used as novel molecular partner for target protein surface. Second, this library can include more than billions of compounds. Thus, hit compounds with strong binding affinities are expected to find. Finally, high-throughput screening with fluorescence activated cell sorter can be adapted to this library, since bead size is similar with cell. In the model compound synthesis, the peptoid synthesis was alternatively conducted with coding material elongation reaction. The cyclic peptoid and coding material were well synthesized. This study demonstrated synthesis of cyclic peptoid OBOC library using tiny beads including billions of compounds. It will be used as platform to find novel hit compounds for target proteins with strong binding affinities.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-140**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mechanical properties of lipid vesicle upon hole formation due to the insertion of antimicrobial peptides

이세린 남소정 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Antimicrobial peptide(AMP) is well-known cell penetrating peptide, containg cationic peptide which have both hydrophobic and hydrophilic properties. Since these amphipathic characteristic, AMP can do membrane attack resulting in pore formation on membrane. In previous study, the AMP induce membrane thining and stiffer to lipid model membrane. However, it is unclear that in living cell, how AMP change cell mechanical properties. For studying this, I used micropipette aspiration which can measure young's modulus of single cell by suction of membrane into pipette. Then, we observed the effect of melittin, one of AMP, to mechanical properties of cells with studying actin change in cell.

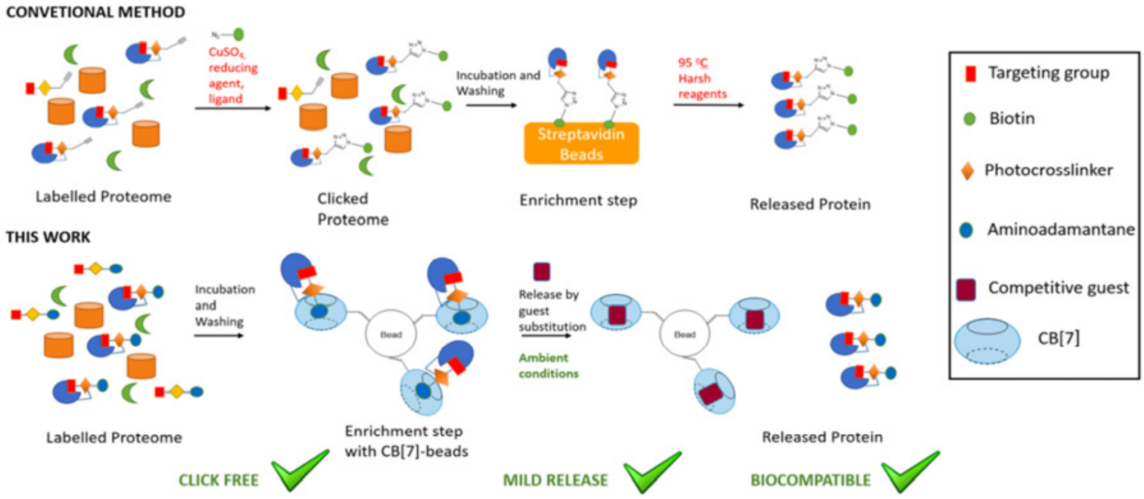
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-141**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Supramolecular Proteomics: Enrichment of Specific Proteins by Use of an Ultrastable Host-guest Complex

James Murray 심재환[1] 이아라[2] 박경민[3] 김기문[4,*]

기초과학연구원 복잡계 자기조립 연구단 [1]POSTECH 시스템생명공학부 [2]포항공과대학교 첨단재료과학부 [3]기초과학연구원 복잡계자기조립연구단 [4]POSTECH 화학과

Proteomics is reliant on the use of enrichment technologies to isolate proteins of interest. Chemical labelling of a specific protein, protein family or functional group with biotin and then capturing on immobilized streptavidin (SA) is a powerful enrichment method. However, it has some limitations: endogenous biotinylated molecules can interfere and the release of the enriched proteins from the solid support usually requires harsh reagents and high temperature. Typically, biotin is 'clicked-on' after protein labelling, but the click reaction requires addition of a large (0.01 - 1 mM) amounts of labeling reagents and can be inefficient in complex media such as a cell lysate. Synthetic alternatives with biotin-SA like affinities until recently have been lacking. Cucurbit[*n*]urils (CB[*n*]) are an emerging technology that can form host-guest complexes with affinities comparable to biotin-SA.[1] We recently described how CB[7] could be used to enrich ferrocene-labeled membrane proteins[2]. Herein, we report how this technology can enrich specific cytoplasmic proteins by use of affinity-based photo-crosslinking. The CB[7] system has several advantages over SA-biotin; namely that a click reaction is not required, the release of the protein is mild and the system is synthetic but biocompatible. References1.Shetty, D.; Khedkar, J. K.; Park, K. M.; Kim, K. *Chem. Soc. Rev.* 2015, *44*, 8747-8761.2.Lee, D. W. et al. *Nat. Chem.* 2011, *3*, 154-159.


CONVETIONAL METHOD
N_3
$CuSO_4$, reducing agent, ligand
Incubation and Washing
Streptavidin Beads
95 °C Harsh reagents
Labelled Proteome
Clicked Proteome
Enrichment step
Released Protein
THIS WORK
Incubation and Washing
Bead
Release by guest substitution
Ambient conditions
Bead
Labelled Proteome
Enrichment step with CB[7]-beads
Released Protein
CLICK FREE
MILD RELEASE
BIOCOMPATIBLE
Targeting group
Biotin
Photocrosslinker
Aminoadamantane
Competitive guest
CB[7]

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-142**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Formation of Extracellular Matrix–adsorbed lipid vesicles and their mechanical properties

김민영 이세린[1,*] 남소정[1,*] 신관우[2,*]

서강대학교 화학 [1]서강대학교 화학과 [2]서강대학교 화학과 및 바이오융합과정

The extracellular matrix (ECM) has important roles in regulating the development, function and homeostasis of all eukaryotic cells. More importantly, ECM provides mechanical stability to cellular membrane. GUV which contain PS lipid can be coated with ECM because of its negative charge. This GUV can be measured by micropipette aspiration. Micropipette aspiration is one of the methods for measuring mechanical properties of cell and vesicle membrane. Area expansion modulus can be calculated. By suction of membrane into micropipette, we can get response or modulus data about mechanical loading on GUV which is coated with ECM. Then, we observed the effect of ECM to mechanical properties of cells.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-143**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Construction and high-throughput screen of an ultra-large bead library for rapid discovery of potent protein binding ligands

이강주 임현석*

POSTECH 화학과

Macrocyclic peptide has been considered as a promising class of protein binding ligands. Macrocyclization offers pre-organized structure compared to their linear counterpart, thus the cyclic molecules can bind more tightly with target protein without major entropy losses. Moreover, they often showed improved cell permeability and proteolytic resistance. To this end, macrocyclic peptides are utilized widely in combinatorial screening strategies. Among them, on-bead screening using one-bead one-compound (OBOC) library is an efficient and economic method. A large number of compounds can be synthesized and screened simultaneously via OBOC approach. In spite of their utility, current on-bead screening methods have critical limitations. Due to relatively large size of the bead (~100 μm), the volume of bead library containing more than 1 million compounds exceeds practical handling capacity. On-bead screening with limited number of diversity yields relatively low hit ratio. In addition, the hit compounds typically show moderate or weak affinity to target proteins.To overcome such limitations, we used much smaller beads (~10 μm) to construct the bead library. In theoretically, the library is capable of containing a tremendous number of diversity over billions in a practical handling volume. As a model system, 150 million-membered 7-mer cyclic peptide library was synthesized on the tiny beads. After screening procedure, the hit beads, that are bound with labeled target protein, can be isolated automatically by fluorescence-activated cell sorting (FACS). This novel on-bead screening technology will facilitate the rapid identification of PPI modulators bearing high-affinity to a target protein.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-144**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dual anticancer effects of DNAzyme on non-small cell lung cancer cells harboring the EGFR mutation

백유미 김동은*

건국대학교 생명공학과

Epidermal growth factor receptor (EGFR) tyrosine kinase inhibitors are the main therapeutic agents used to treat non–small-cell lung cancer (NSCLC) patients harboring EGFR-activating mutations. Most of EGFR gene mutations in NSCLC patients have been commonly observed in the exon 19, which often contains deletion of amino acids from 746 to 750. This somatic mutation leads to expression of the mutant EGFR on the lung epithelial cell surface and results in continuous cell division by uncontrolled kinase activity. Thus, it is important to inhibit expression of mutant EGFR for suppression of cancer cell proliferation in NSCLC patients. In this study, we designed a DNAzyme to inhibit expression of mutant EGFR containing exon 19 deletions (EGFR19Δ). The DNAzyme specifically cleaved target RNA in vitro. Anticancer effect of DNAzyme transfected into the gefitinib-resistant lung cancer cells harboring EGFR19Δ was observed through cell viability assay and flow cytometry analysis. DNAzyme decreased protein expression of EGFR and its downstream signal transduction pathway, as observed by western blot. Unexpectedly, DNAzyme with reverse sequences (i.e. scrambled Dz, used as a negative control) also showed anticancer efficacy by lowering cell viability in a dose-dependent manner. We suggested a possible non-specific effect caused by the CpG sequences in oligonucleotides transfected in the epithelial cells. This hypothesis was supported by observation that the CpG-rich DNA resulted in decreased viability of lung cancer cell, while the oligo dT DNA did not. Therefore, our results indicate that ex19del Dz is effective to decrease lung cancer cell proliferation by specific cleavage of mutant EGFR RNA as well as non-specific cytotoxicity caused by CpG DNA sequences.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-145**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mirror DNA nanostructures for anticancer drug delivery

김경란 안대로[1,*]

연세대학교 화학과 [1]한국과학기술연구원(KIST) 테라그노시스연구단

Our new approach provides an alternative strategy for tumor-specific delivery of anticancer drugs and highlights the promising potential of the mirror DNA nanostructures as a novel drug delivery platform.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-146**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Hydrolysis of metabolic chemical reporter analog PNP-6AzGlcNAc by O-GlcNAcase

김은주

대구대학교 과학교육학부/화학교육과

6-Azido-6-deoxy-N-acetylglucosamine (6AzGlcNAc) was recently introduced as a new selective metabolic chemical reporter (MCR) for labeling O-GlcNAc-modified proteins in cells. To investigate whether O-6AzGlcNAc is readily cleaved by O-GlcNAcase (OGA), the enzyme responsible for removing the O-GlcNAc modification, we synthesized PNP-6AzGlcNAc. This analog mimics O-GlcNAc and can be used in vitro to define the kinetic parameters for OGA thereby defining whether O-6AzGlcNAc can be considered as appropriate tool to monitor O-GlcNAc dynamics in cells. OGA and PNP-6AzGlcNAc yielded kinetics similar to those with the enzyme and PNP-GlcNAc suggesting that an azido-modification at the GlcNAc C6 position does not significantly alter OGA's behavior compared with its native substrate.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-147**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

YjfN activates DegP, a major periplasmic protease in E. coli

김성재 김석희*

서울대학교 화학부

Bacterial periplasm possesses hundreds of proteins, and many of them are still remain elusive. Here, we report a function of YjfN, a previously unknown periplasmic protein. We proved that it primarily acts as an activator for DegP, a major protease in E. coli periplasm. Interestingly, while activating DegP, YjfN is rapidly degraded because of its extraordinary structural features. This is the first time to discover the protein that is degraded while activating an enzyme. The function of YjfN may give us more profound understanding of protein function.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-148**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

An investigation of cell penetrating activity on bundle dimers of amphipathic helical peptide by alternating cationic residues

최윤화 유재훈*

서울대학교 화학교육과

Dimeric bundles, connected by two disulfide bonds, could be formed by oxidation of Cys residues of the monomeric α-helical LK peptide, sequenced as Ac-LKKLCKLLKKCLKLAG-NH2.While these bundles have shown highly efficient cell penetrating ability relative to Tat or R9, well-known cell penetrating peptide (CPP), thus, they are easily get into eukaryotic cells at their low nano-molar concentrations. Since the LK peptide is mainly composed of Lys and Leu residues, only primary amines in Lys residues are cationic groups in hydrophilic face of the dimer bundle. In order to know roles of these cationic residues upon cell penetrating ability, we did exchange Lys residues to Arg or His residues to make mutant bundle dimers. The fluorescent labelled mutant bundles and fluorescence-activated cell sorting (FACS) experiments using HeLa cells revealed that Arg-mutated dimer possesses compatible cell penetrating ability, while His-mutant bundle showed much lower ability in comparison with the original dimer bundles. Probably, positively charged cationic residues might be the most important factor for cell penetrating ability of dimer bundles. Further investigation is reqired to elucidate more detailed roles of these cationic residues upon cell penetrating ability of the bundle dimers.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-149**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Smenospongidine suppresses the proliferation of multiple myeloma cells by promoting CCAAT/enhancer-binding protein homologous protein-mediated β-catenin degradation

박서영 오상택*

국민대학교 바이오발효융합학과

Abnormal up-regulation of β-catenin expression is associated with the development and progression of multiple myeloma and is thus a potential therapeutic target. Here, we screened cell-based natural compounds and identified smenospongidine, a metabolite isolated from a marine sponge, as an antagonist of the Wnt/β-catenin signaling pathway. Smenospongidine promoted the degradation of intracellular β-catenin that accumulated via Wnt3a or 6-bromoindirubin-3′-oxime, an inhibitor of glycogen synthase kinase-3β. Consistently, smenospongidine down-regulated β-catenin expression and repressed the levels of β-catenin/T-cell factor-dependent genes such as axin2, cyclin D1, and c-myc in RPMI-8226 multiple myeloma cells. Smenospongidine suppressed proliferation and significantly induced apoptosis in RPMI-8266 cells. In addition, smenospongidine-induced β-catenin degradation was mediated by up-regulating CCAAT/enhancer-binding protein homologous protein (CHOP). These findings indicate that smenospongidine exerts its anti-proliferative activity by blocking the Wnt/β-catenin signaling pathway and may be a potential chemotherapeutic agent against multiple myeloma.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-150**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Drug discovery through reverse quantitative structure-retention relationships and molecular simulation

ZUVELAPETAR PHAN THI HONG THAM[1] 유준[*] 이명기[2] Mariusz Belka[3] Tomasz Bączek[3]

부경대학교 화학공학과 [1]부경대학교 의생명기계전기융합공학협동과정 [2]부경대학교 의공학과 [3]Department of Pharmaceutical Chemistry, Medical University of Gdańsk

In this work, a proof of concept of a methodology for design and screening of novel drugs with strong antitumor activity and selectivity towards CA isoenzyme IX (CAIX). Pairs of stereoisomers of 14 sulfonamide derivatives were used to develop a Quantitative structure-retention relationships (QSRR) model for prediction of their lipophilicity. Developed model was inverted through numerical optimization maximizing it. Corresponding optimal values of molecular descriptors were screened against a database of compounds, and ten new drug candidates were identified. Molecular Dynamics (MD) and Quantum Mechanics (QM) simulations were also performed. 5-(1-naphthalen-1-yl-1,2,3-triazol-4-yl)thiophene-2-sulfonamide (9FK) was used as a reference. Upon simulation of 9FK in complex with CAIX, the system conserved the all the main binding features identified experimentally. Substantial theoretical evidence is presented in order to describe the interactions between CAIX and the compounds. They exhibited superior interactions in both the hydrophobic and hydrophilic regions of CAIX, as well as stability in comparison to CAIX-9FK. Future work associated with the methodology involves synthesis and testing activities of the new compounds.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-151**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

NMR study of type III antifreeze protein from *Zoarces elongates Kner*

최서리 이애리 이준화[*]

경상대학교 화학과

Antifreeze proteins (AFPs) are found in a variety of cold-adapted (psychrophilic) organisms to promote survival at subzero temperatures by binding to ice crystals and decreasing the freezing temperature of body fluids. One of most widely studied classes of AFPs is the type III from arctic fish such as the ocean pout and Japanese notched-fin eel pout. The type III AFPs are small globular proteins that consist of one α-helix, three 3_{10}-helices, and two β-strands. The type III AFPs have been categorized into two subgroups, quaternary-amino-ethyl (QAE) and sulfopropyl-Sephadex-binding (SP), based on differences in their isoelectric points. The QAE proteins can be further divided into two subgroups, QAE1 and QAE2. QAE2 isoforms can slow, but not stop, the growth of ice crystals by binding to pyramidal ice planes. The other group (QAE1) binds both pyramidal and primary prism planes and is able to halt the growth of ice.In this study, we have investigated backbone dynamics analyses of four kinds of type III AFPs from Japanese notched-fin eel pout (Zoarces elongates Kner), wt AFP8 (QAE1), V20A_AFP8 , V20G_AFP8, AFP8_di and AFP8_tri at various temperatures. We also characterized the structural/dynamic properties of the ice-binding surfaces by analyzing the temperature gradient of the amide proton chemical shift and its correlation with chemical shift deviation from random coil. This study provides insight into the molecular basis of ice-binding and antifreezing activities of type III AFP isoforms

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-152**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Importance of each secondary structure of IF(insertion-in-flap) in amyloid formation of FKBPIF-L23-hIAPP fusion protein

윤소영* 이경희

세종대학교 화학과

Human islet amyloid polypeptide (hIAPP) protein of the type II diabetes patient rapidly forms amyloid fibrils as other aggregation-prone proteins such as synuclein as well as aβ protein. In the previous study, FKBPIF(and F36VIF)-L23-hIAPP fusion protein exhibited the higher tendency to accelerate amyloid fibril formation than SlyD*-L23-hIAPP. In this study, 4 different deletion mutations were introduced in the IF(insertion-in-flap) domain of FKBPIF-L23-hIAPP fusion system. Each deletion mutant protein overexpressed by IPTG in E.coli were further purified by Ni2+- affinity chromatography and checked the amyloid formation by measuring Thioflavin T fluorescence. Here we discuss the importance of each secondary structure of IF domain in regulating amyloid formation of hIAPP in vitro.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-153**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Inhibitory RNA Aptamers of Tau Oligomerization and Their Neuroprotective Roles against Proteotoxic Stress

김지현 김은경 이민재*

서울대학교 의과대학 생화학교실

Alzheimer's disease is characterized by aggregation of two hallmarks, tau and amyloid beta. Among these misfolded proteins, several studies show that tau aggregation trigger formation of amyloid plaques. Moreover, newly came out researches said that oligomeric tau is more harmful than neurofibrillary tangle (NFT). Until now small molecule tau aggregation inhibitors have been under investigated as potential therapeutic agents against Alzheimer disease. In this study, to find inhibitor of tau oligomerization, we used a systematic evolution of ligands using the exponential enrichment (SELEX) procedure. Here we selected specific anti- tau RNA aptamer 76% homology as named Tau-1. In the binding affinity test, we showed that Tau-1 bounds to tau dose dependently compared with control group. Tau-1 effectively inhibits tau oligomerization, as measured by *in vitro* tau aggregation assay and thioflavin S assay. We confirmed that Tau-1 doesn't have any effects on biological events of tau using *in vitro* transcription/translation. In addition, inhibition of tau oligomerization in cultured cells is also confirmed by using HEK 293 TREX Tau cell and Tau-Bifc cell. To demonstrate inhibitory ability of Tau-1, we identified proteasome and autophagy activity which were not changed. Thus, our study identifies inhibitory Tau-1 aptamer to facilitate inhibition of proteotoxic protein aggregation and may have protential as therapeutic agents for AD pathogenesis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **BIO.P-154**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The Arg/N-end rule pathway as positive regulator of autophagic flux & proteotoxic protein degradation

이지영 이정훈 이민재*

서울대학교 의과대학 생화학교실

A protein has the N-terminal amino acid which is an essential determinant of ubiquitination and subsequent proteasomal degradation in the N-end rule pathway. We show here that blocking the arginylation branch of the N-end rule pathway (Arg/N-end rule pathway) significantly impaired the fusion of autophagosomes with lysosomes by using para-chloroamphetamine (PCA) as a specific inhibitor of the Arg/N-end rule pathway. Under ER stress, the N-terminal arginylation of the ER heat shock protein HSPA5 (HSPA5/GRP78/BiP) that originally targets cargo proteins is moved out by ATE1-encoded Arg-tRNA-protein transferases in the cytosol, along with p62, to the autophagosome. At the late step of autophagy, proteasomal degradation of N-terminally arginylated HSPA5 (Arg-HSPA5) could role as a critical checkpoint for the proper progression of autophagic flux in the cells. Cells continuously treated with PCA exhibited upregulated levels and aggregation of autophagic markers such as LC3, p62, and proteotoxic proteins like tau and huntingtin. Treatment the Arg/N-end rule inhibitor in cells enhanced proteotoxic stress-induced cytotoxicity. Quantitative mass spectrometry with SILAC revealed that PCA significantly makes some changes in various biological pathways such as primarily cellular responses to stress, autophagic responses. Thus, the Arg/N-end rule pathway may play a significant role of positively regulating autophagic flux under a number of stress conditions for protecting cells from harmful influences of proteotoxic protein accumulation.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **BIO.P-155**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Deletion of the N-terminus tail of alpha3 increases mammalian proteasome activity by "Open-Gate"

김선무 최원훈 이민재*

서울대학교 의과대학 생화학교실

Proteasomes degrade misfolded or damaged protein by proteolysis. The proteasome is the ~2.5 MDa holoenzyme complex consisting of two distinguishable the 19-subunit regulatory particle (RP, also known as the 19S) and the 28-subunit core particle (CP, also known as the 20S). CP is a cylindrical complex composed of four stacked rings. The internal two rings are made of seven beta-subunits (beta1-7) that contain catalytic sites. And the outer two rings are made of seven alpha-subunits (alpha1-7). The alpha-rings function as the "gate" when substrates enter to the barrel. When in the closed form, the axial substrate translocation channel of the CP is topologically blocked by the convergent N-termini of alpha subunits. To probe the role of channel gating in mammalian proteasomes, we have deleted the N-terminal tail of alpha 3. Here we show alpha3deltaN proteasomes are intact but hyperactive. It shows enhanced activity in three catalytic cites by measure the hydrolysis of fluorogenic peptide substrates. Polyubiquitinated Sic1 also showed enhanced degradation by purified alpha3deltaN proteasomes. Stable cells which are dominant negatively expressing the hyperactive proteasomes showed markedly elevated degradation of established proteasome substrates. And they were viable and highly resistant to oxidative stress. Potentially toxic proteins such as tau exhibited reduced accumulation and aggregate formation. These result provides that regulation of CP gate may function as the critical rate-limiting step in proteasomal degradation, and that opening the CP gate may be an effective strategy to reduce levels of aberrantly overexpressed or misfolded proteins in cells.

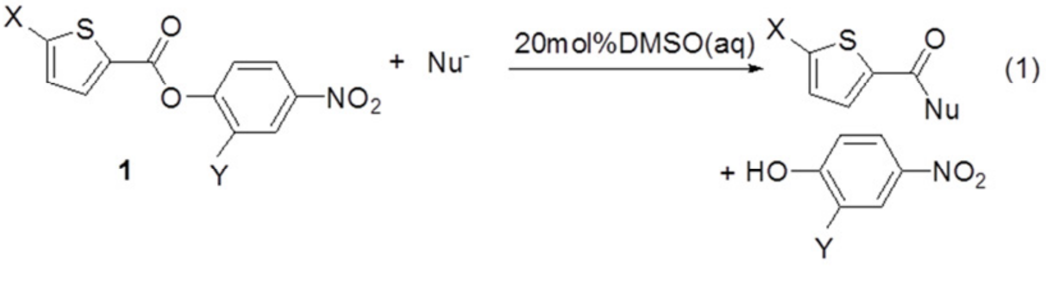
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-156**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Reactions of Aryl 5-substituted-2-Thiophenecarboxylates Promoted by4-Z-$C_6H_4O^-$/4-Z-C_6H_4OH in 20 mol % DMSO(aq). Effect of Nucleophile on Acyl-Transfer Reaction

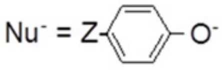
변상용* 조봉래[1]

부경대학교 화학과 [1]대진대학교 화학과

Nucleophilic substitution reactions of 5-$XC_4H_2(S)C(O)C_6H_3$-2-Y-4-NO_2 (1) promoted by 4-Z-$C_6H_4O^-$/4-Z-C_6H_4OH in 20 mol % dimethyl sulfoxide (DMSO)(aq) have been studied kinetically. The reactions exhibitedsecond-order kinetics with $\beta_{acyl} = -2.52$ to -2.83, $\rho(x) = 2.81–3.16$, $\beta_{nuc} = 0.88–0.04$ and $\beta_{lg} = -0.94$, respectively. The results have been interpreted with an addition–elimination mechanism in which the nucleophilic attack occurs in the rate-determining step. Comparison with existing data reveals that the ratedetermining step changes from the second to the first step by the change in the nucleophile from $R_2NH/R_2NH_2^+$ to 4-Z-$C_6H_4O^-$/4-Z-C_6H_4OH



X = H (**a**), MeO (**b**), Me (**c**), Cl (**d**), NO_2 (**e**); Y= H (**a'**), MeO (**b'**), Cl (**c'**), CF_3(**d'**), NO_2 (**e'**)



; Z = H, MeO, Me, Cl, CN

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-157**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Zinc Enolate/Sulfinate Prepared from a Single-Run Reaction Using Zinc Dust with O-Tosylated 4-Hydroxy Coumarin and Pyrone

김종성 주성류 김승회*

단국대학교 화학과

The preparation of new zinc complexes, 2-oxo-2H-chromen-4-yloxy tosylzinc (I) and 6-methyl-2-oxo-2H-pyran-4-yloxy tosylzinc (II), were demonstrated by the oxidative addition of readily available zinc dust into the corresponding 4-tosylated coumarin (A) and pyrone (B), respectively.Of special interest, the thus-obtained zinc complexes showed an electrophile-dependent reactivity. The subsequent coupling reactions of I and II with a variety of acid chlorides provided the O-acylation product in moderate yields. More interestingly, it should be emphasized that the thus-prepared zinc complexes (I and II) functioned both as zinc enolate and zinc sulfinate, providing C(3)-disubstituted product (b) and sulfone (c), respectively, from a single-run reaction when I or II was treated with benzyl halides. Even though somewhat low yields were achieved under the non-optimized conditions, the novel zinc complexes present another potential application for zinc reagents.

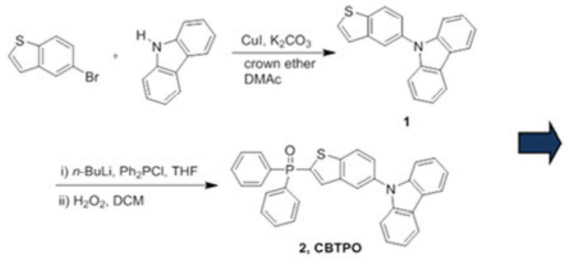
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-158**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

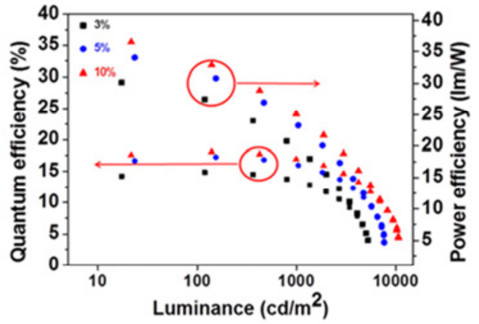
Synthesis and characterization of novel benzothiophene derivative as a host material for blue phosphorescent OLEDs

서초현 서성용*

부경대학교 화학과

An organic compound having carbazole, benzothiophene, and phosphine oxide moieties, (5-(9*H*-carbazol-9-yl)benzo[*b*]thiophen-2-yl)diphenylphosphine oxide (CBTPO), was synthesized and employed as a blue host material to harvest triplet excitons from blue triplet emitters. The CBTPO material is a bipolar host material because it includes carbazole and diphenylphosphine oxide charge transport units with both a high triplet energy of 2.76 eV and a high quantum efficiency of 19.1% in blue phosphorescent device.





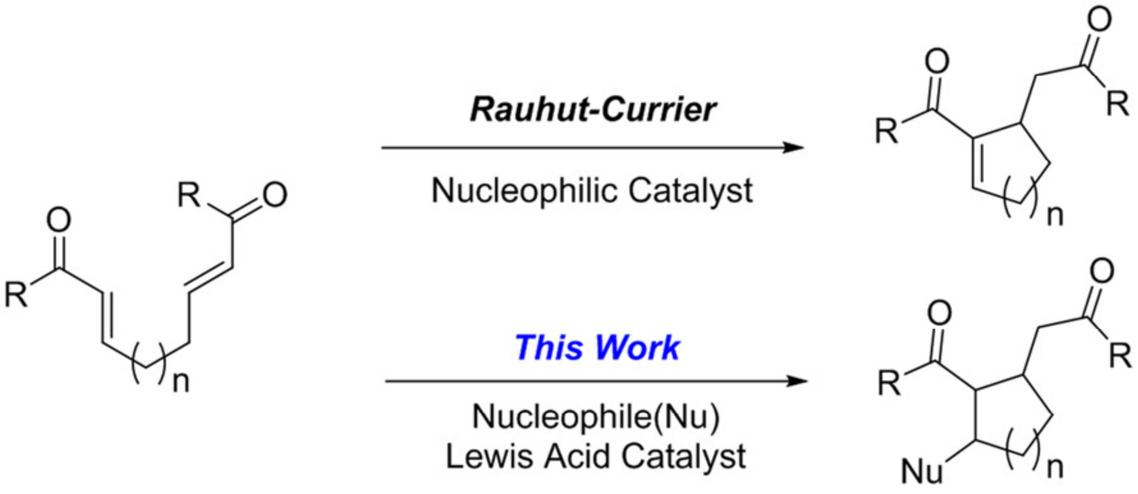
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-159**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Indium triflate-catalyzed tandem intramolecular conjugate addition with primary alcohol to α,β-bisenones

전민석 서성용*

부경대학교 화학과

We conducted tandem intramolecular conjugate addition of α,β-bisenones to primary alcohols activated by sodium hydride in order to synthesize a 1,2,3-trisubstituted six membered ring as one-pot reaction catalyzed by Indium triflate. After optimizing reaction conditions, we examined electronic effect of substrate by changing substituent of α,β-bisenones and nucleophiles from electron-withdrawing group to electron-donating group in detail.



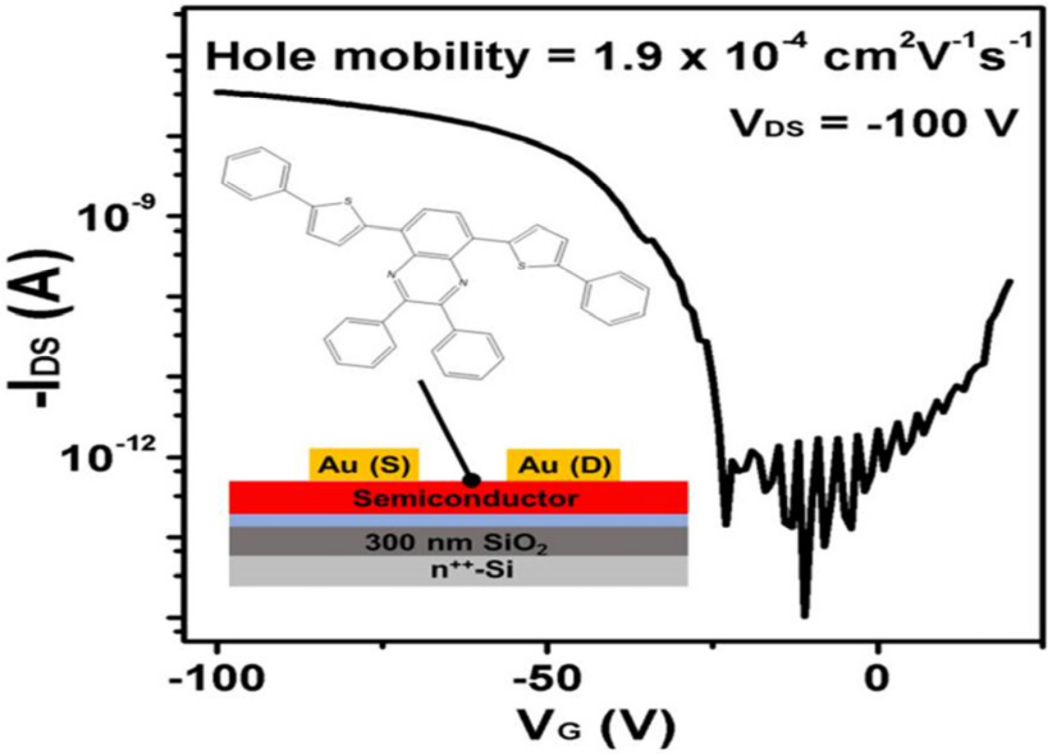
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-160**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Characterization of Quinoxaline Derivative as Organic Semiconductors for Organic Thin-Film Transistors

김평강 **machireddy rajeshkumar reddy*** 서성용*

부경대학교 화학과

Three new quinoxaline-based derivatives, end-functionalized with 2,3,5,8-tetraphenyl (3), 2,3-diphenyl-5,8-di(thiophen-2-yl) (4), and 2,3-diphenyl-5,8-bis(5-phenylthiophen-2-yl) (5) were synthesized, characterized, and incorporated as organic semiconductors in top-contact/bottom-gate organic thin-film transistors (OTFTs). Thermal, optical, and electrochemical properties of the newly developed compounds were fully investigated. For the fabrication of thin films of all three compounds, solution-shearing (SS) and vacuum deposition method were employed. Thin films of compound 5 showed p-channel characteristics with hole mobilities as high as 2.6 × 10^{-5} cm^2/Vs and current on/off ratio of 1.8 × 10^5 via solution process and 1.9 × 10^{-4} cm^2/Vs and current on/off ratio of 3.5 × 10^6 via vacuum deposition.


Hole mobility = 1.9 x 10^{-4} cm^{2}V^{-1}s^{-1}
V$_{DS}$ = -100 V
10^{-9}
10^{-12}
-I$_{DS}$ (A)
S
N
N
S
Au (S)
Au (D)
Semiconductor
300 nm SiO$_2$
n^{++}-Si
-100
-50
0
V$_G$ (V)

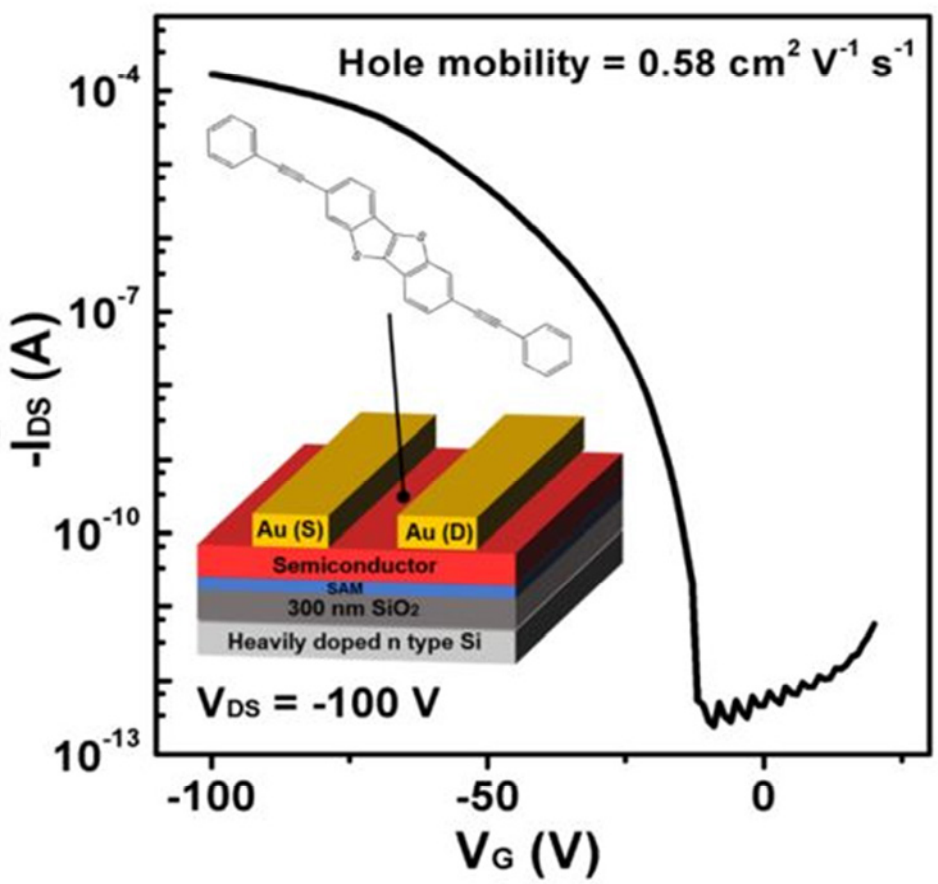
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-161**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Characterization of 2,7-Diethynylbenzo[*b*]benzo[4,5]thieno[2,3-*d*]thiophene Derivative as Organic Semiconductors for Organic Thin-Film Transistors

machireddy rajeshkumar reddy 서성용*

부경대학교 화학과

New benzo[*b*]benzo[4,5]thieno[2,3-*d*]thiophene derivatives were synthesized and characterized as organic semiconductors in top-contact/bottom-gate organic thin-film transistors (OTFTs). Newly developed materials were fully characterized by thermogravimetric analysis, differential scanning calorimetry, UV-vis spectroscopy, cyclic voltammetry, and density functional theory calculation. New compounds were vacuum-deposited as thin films, and investigated by X-ray diffraction (XRD) and atomic force microscopy (AFM). Thin-film transistors based on compound 1 showed decent p-channel characteristics with carrier mobility as high as 0.58 cm^2 V^{-1} s^{-1} and on/off ratio of 10^6 – 10^9. Thin film microstructure and surface morphologies hasve been correlated with the corresponding device performance.


Hole mobility = 0.58 cm^2 V^{-1} s^{-1}
10^{-4}
10^{-7}
10^{-10}
10^{-13}
$-I_{DS}$ (A)
Au (S)
Au (D)
Semiconductor
SAM
300 nm SiO_2
Heavily doped n type Si
V_{DS} = -100 V
-100
-50
0
V_G (V)

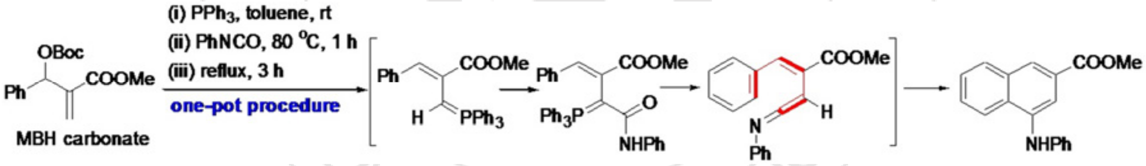
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-162**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Aminonaphthalenes from Morita-Baylis-Hillman Carbonates *via* 6π-Electrocyclization of Ketenimine Intermediates

민범규 노화정 김재녕*

전남대학교 화학과

Various aminonaphthalenes have been synthesized from Morita-Baylis-Hillman (MBH) carbonates and isocyanates in one-pot reaction in moderate yields *via* sequential formation of MBH ylide, the reaction of MBH ylide and isocyanate to form amide ylide, formation of ketenimine intermediate by liberation of triphenylphosphine oxide, and 6π-electrocyclization.



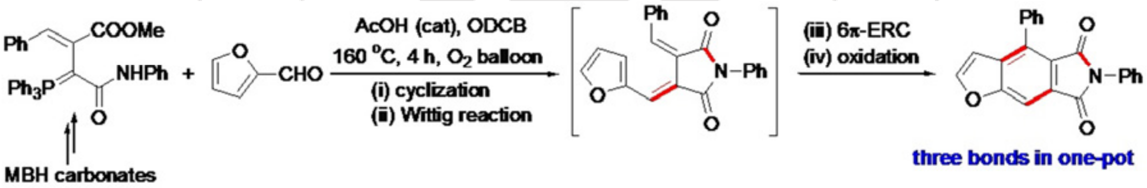
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-163**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

An Expedient Synthesis of Arene-Fused Phthalimides from Morita-Baylis-Hillman Carbonates

민범규 노화정 김재녕*

전남대학교 화학과

Various arene-fused phthalimides have been synthesized *via* one-pot reaction of amide ylides and aromatic aldehydes in the presence of AcOH in 1,2-dichlorobenzene (ODCB) at 160 °C. The reaction involved 6π-electrocyclization reaction of conjugated triene bearing an aromatic double bond and a following aerobic oxidation process.



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-164**

발표분야: 유기화학

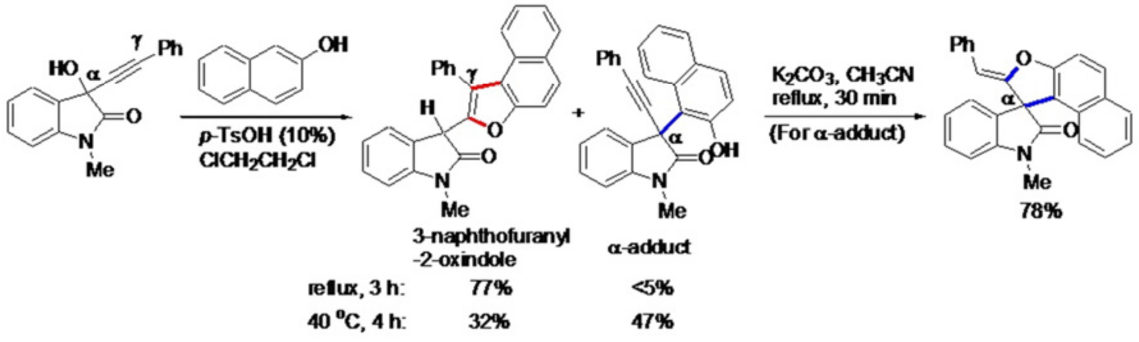
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-Pot Synthesis of 3-Naphtho[2,1-*b*]furanyl-2-oxindoles from 3-(Arylethynyl)-3-hydroxyindolin-2-ones and 2-Naphthols

노화정 임진우 김재녕[*]

전남대학교 화학과

3-Naphthofuranyl-2-oxindoles have been synthesized by the reaction of 3-(arylethynyl)-3-hydroxyindolin-2-ones and 2-naphthols *via* Friedel-Crafts reaction and a following Michael type 5-*exo-dig* cyclization. In addition, dihydrofuranyl-spirooxindoles were synthesized from 3-(*ortho*-hydroxyaryl)-2-oxindoles by base-catalyzed cyclization reaction.



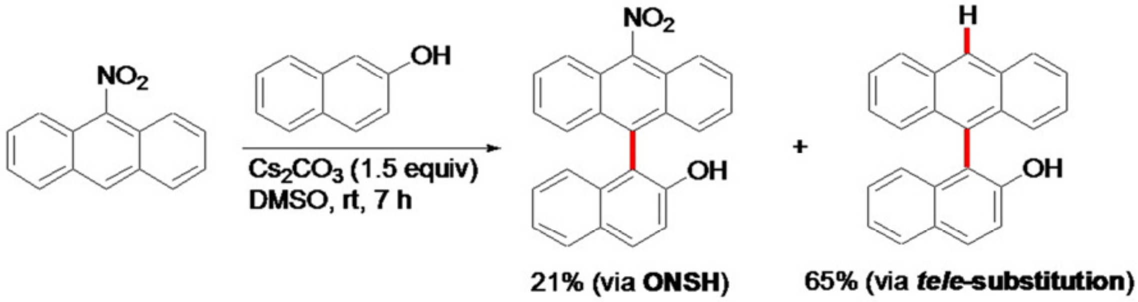
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-165**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Nucleophilic Aromatic *tele*-Substitution of Hydrogen of 9-Nitroanthracene with 2-Naphthols and Phloroglucinol

김수연 임진우 김재녕*

전남대학교 화학과

A selective nucleophilic aromatic *tele*-substitution reaction has been observed in the reaction of 9-nitroanthracene with 2-naphthols, 1,3-cyclohexanediones and phloroglucinol. The corresponding nitroanthracene derivatives, obtained by an ONSH (oxidative nucleophilic substitution of hydrogen) process, were formed in variable yields as minor products depending on the substrates.



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-166**

발표분야: 유기화학

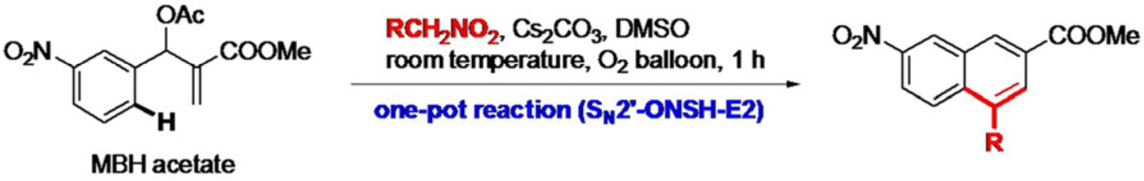
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-Pot Synthesis of Nitronaphthalenes from Morita–Baylis–Hillman Acetates and Primary Nitroalkanes *via* Sequential S_N2'-Intramolecular Oxidative Nucleophilic Substitution of Hydrogen-E2 Elimination

김수연 민범규 김재녕*

전남대학교 화학과

Various poly-substituted naphthalenes bearing a nitro group at 6- or 7-positions have been synthesized from Morita-Baylis-Hillman (MBH) acetates and primary nitroalkanes in moderate yields in one-pot procedure. The reaction involved three consecutive processes: an introduction of nitroalkane in S_N2' fashion, an intramolecular aerobic ONSH (oxidative nucleophilic substitution of hydrogen) reaction, and a final E2 elimination of HNO_2.



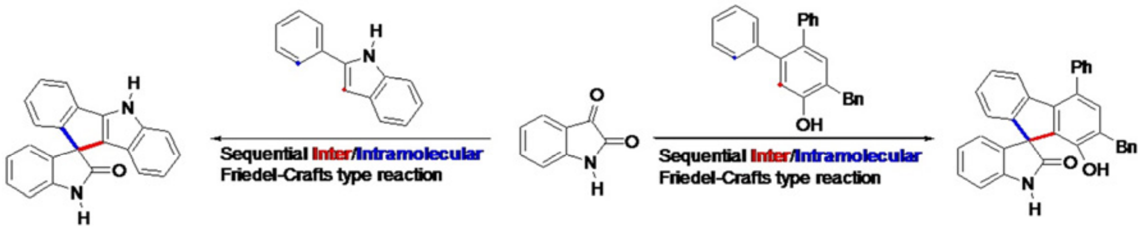
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-167**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-Pot Synthesis of Spirofluorenyl- and Spiroindeno[1,2-*b*]indolyloxindoles *via* Sequential Inter- and Intramolecular Friedel–Crafts Reactions

임진우 김수연 김재녕*

전남대학교 화학과

Various spirofluorenyl oxindoles and spiroindeno[1,2-*b*]indolyl oxindoles have been synthesized in good yields in one-pot reaction by $TiCl_4$-catalyzed sequential inter- and intramolecular Friedel–Crafts reactions of isatins with *meta*-arylphenols and 2-arylindoles in 1,2-dichloroethane.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-168**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Photo-induced Copper Catalyzed Cyanation of Aromatic Halides at Room Temperature

김기철 홍순혁[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Photo-induced copper catalyzed cyanation of aromatic halides was developed under mild conditions. The developed reaction is applicable to various functional groups including primary amines and carboxylic acids. Mechanistic investigations, such as copper intermediates, light-dark experiment, radical scavenger studies, and kinetic study suggest that the reaction between aryl halide and an excited copper(I) cyanide catalytic intermediate occurs via SET process.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-169**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient Preparation of Asymmetrical Ureas from Carbamoylimidazole via Activation of Diethylaluminum Chloride

김희권

전북대학교 의학전문대학원/핵의학교실

Urea is common chemical structure in various natural compounds and biologically active compounds. In additions, ureas have numerous applications in the field of plant growth regulators, selective antagonist, dyes, detergent additives. Herein, novel synthetic method for the preparation of asymmetrically substituted ureas from amines is described. The carbamoylimidazole compounds were readily obtained by the reaction of 1,1-carbonyldiimidazole with several amines, and they were treated with diethylaluminum chloride for the activation to afford corresponding urea structures. This synthetic protocol containing activation by diethylaluminum chloride was allowed to prepare diverse trisubstituted and tetrasubstituted ureas with high yield.

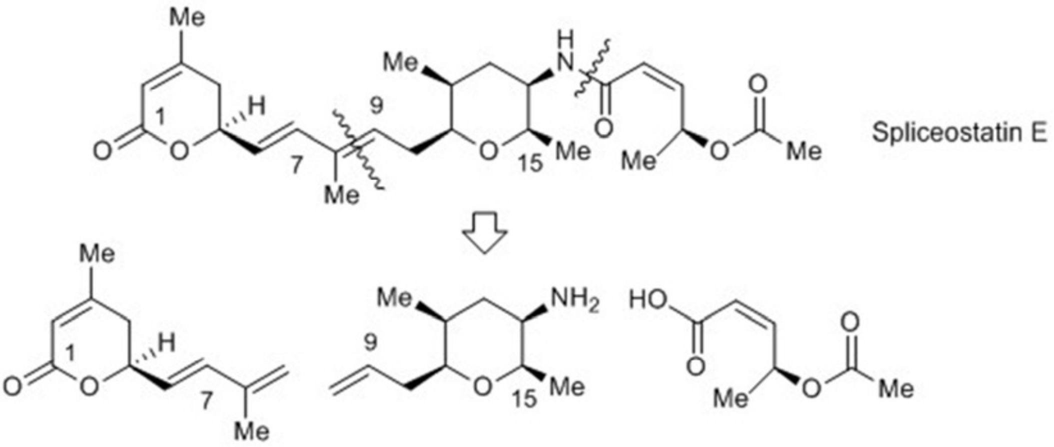
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-170**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Studies towards the Total Synthesis of Spliceostatins

강한영* 임태일

충북대학교 화학과

Spliceostatins, possessing splicing inhibitory activity, are a series of structurally complex molecules with implications of anticancer drug development. Spliceostatin E, shown below, is simplest one in structure that belongs to spliceostatins. This compound has a substituted tetrahydropyran ring, which is a common core part found in a variety of natural products. We have investigated to the efficient synthetic routes for the substituted tetrahydropyran rings. We will present our recent efforts to prepare the core tetrahydropyran ring part of the Spliceostatin E with the aim of achieving the total synthesis of this natural product.



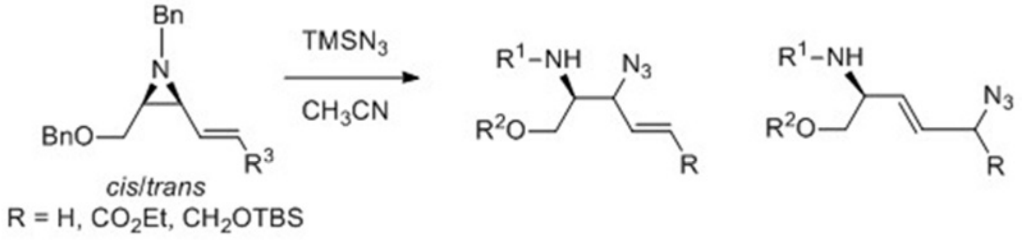
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-171**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ring-opening Reactions of Alkenylaziridines with Trimethylsilyl Azide

강한영* 정소리

충북대학교 화학과

Attack of Nitrogen nucleophiles such as amines and nitrogen heterocycles always occurs at the C-2 position of alkenylaziridines (the position linked to the vinyl group) and this is an excellent way to obtain 1,2-diamino products. Because introducing an azido group is also an efficient way to install an amino group, we decided to investigate the ring-opening reaction of alkenylaziridines by azides. We chose N benzyl protected alkenylaziridines, shown below, as representative substrates for the investigation of these ring-opening reactions. Because the ring-opening reactions proceeded efficiently under Lewis acidic conditions, trimethylsilyl azide (TMSN$_3$) was selected as a nucleophilic reagent. Allylic azides, the products being formed after the nucleophilic ring opening, have feasibility to undergo the allylic azide rearrangement. The products and their distributions resulting from the nucleophilic ring-opening of alkenylaziridines will be presented.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-172**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Novel solid-phase synthetic method for trisubstituted 1*H*-pyrazolo[3,4-*d*]pyrimidine derivatives

허윤정 전문국[1,*]

고려대학교 화학과 [1]한국화학연구원 의약화학연구센터

The coupling of 1-aryl-4,5-dihydro-4-oxo-1*H*-pyrazolo[3,4-*d*]pyrimidine-6-carboxylic acid with a primary alkylamine-loaded AMEBA (Acid sensitive MEthoxy BenzAldehyde) resin, a BOP (benzotriazol-1-yloxytris(dimethylamino)phosphonium hexafluorophosphate)-mediated amination reaction, and cleavage from the solid support yielded *N*-alkyl-4-alkylamino-1-aryl-1*H*-pyrazolo[3,4-*d*]pyrimidine-6-carboxamide derivatives. The progress of the reactions on solid phase was monitored through ATR-FTIR spectroscopy and was compared with representative solution-phase surrogates.

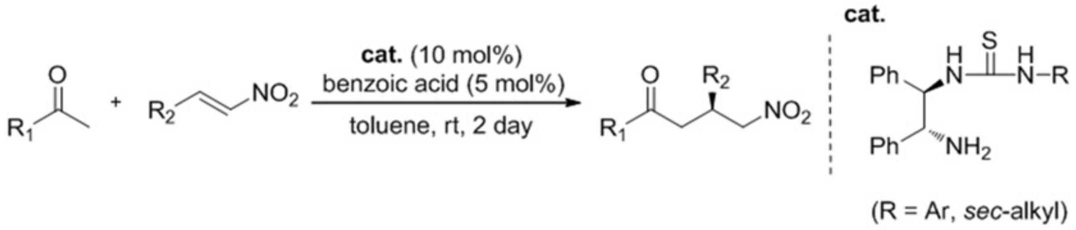
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-173**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Organocatalytic asymmetric Michael additions of aromatic ketones to α,β-unsaturated nitro compounds

남시훈 하덕찬*

고려대학교 화학과

The organic catalyst (R,R)-1,2-diphenylethylenediamine was developed as a chiral bifunctional organocatalyst and successfully applied to asymmetric Michael additions of aromatic ketones to α,β-unsaturated nitro alkene compounds (up to 96% yield, 98% ee) under neutral condition. Systematic investigations on the catalytic mechanism revealed that the role of the thiourea moiety. Generally, isopropyl substituted thiourea catalyst in neutral condition give high chemical yields and enantioselectivities. (Scheme 1)



Scheme 1

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-174**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Endoplasmic Reticulum-Localized Ir(III) Complexes as Photodynamic Therapy Agents via Protein Modifications

남정승 강주혜[1] 임미희[1,*] 권태혁[2,*]

UNIST 화학과 [1]UNIST 자연과학부/화학과 [2]UNIST 친환경에너지 공학부

Protein inactivation by reactive oxygen species (ROS) such as singlet oxygen ($^1O_2$) and superoxide radical ($O_2^{\bullet-}$) is considered to trigger cell death pathways associated with protein dysfunction; however, the detailed mechanisms and direct involvement in photodynamic therapy (PDT) have not been revealed. Herein, we report Ir(III) complexes designed for ROS generation through a rational strategy to investigate protein modifications by ROS. The Ir(III) complexes are effective as PDT agents at low concentrations with low-energy irradiation ($\leq$ 1 J cm^{-2}) because of the relatively high $^1O_2$ quantum yield (> 0.78), even with two-photon activation. Furthermore, two types of protein modifications (protein oxidation and photo-cross-linking) involved in PDT were characterized by mass spectrometry. These modifications were generated primarily in the endoplasmic reticulum and mitochondria, producing a powerful effect for cancer cell death. Consequently, we present a plausible biologically applicable modality that utilizes rationally designed photoactivatalbe Ir(III) complexes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-175**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Practical Synthesis of Thioesters Using Carbon Monoxide Gas from Oxalyl Chloride

김희권

전북대학교 의학전문대학원/핵의학교실

Thioesters are important chemical units in a various biologically active compounds, and they have been utilized as synthetic intermediates in acyl transfer reactions. They are also important compounds from organic synthetic area. Even though, various traditional synthetic methods such as condensation reaction of carboxylic acids with thiols or metal thiolates have been developed, they have some weakness. Here, we describe simple and facile method for the preparation of thioesters using reactive carbon monoxide gas. Carbon monoxide gas was readily obtained through Zn-mediated reduction of oxalyl chloride and was utilized to Pd-catalyzed thioesterification. After examination of conditions of thioesterification reaction, aryl halides were treated with thiols in the presence of oxalyl chloride, pd catalyst, Xantphos in order to produce corresponding thioesters. In novel synthetic methodology using carbon monoxide gas generated from oxalyl chloride, a variety of desired thioesters was prepared in high yield.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-176**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly Selective Cyanide Detection by Dual Optical Indocyanine Probe

박석안 김해조*

한국외국어대학교 자연과학대학 화학과

We report a dual optical probe based on N-hydroxyethylindocyanine for the selective detection of cyanide in water. The probe exhibited a dramatic red-to-colorless optical change and a fluorescence on–off response in the visible region, displaying high selectivity toward cyanide over other various anions and Cys with a micromolar limit of detection (LOD = 2.0 μM) in an aqueous buffer. Furthermore, the probe underwent a reversible reaction with the probe-cyanide ion adduct in the presence of Hg(II), of which optical changes were easily detected by direct visualization.References1. Park S, Kim H-J. Reaction-based chemosensor for the reversible detection of cyanide and cadmium ions. Sens Actuators B 2012, 168, 376.2. Park S, Kim H-J. Highly activated Michael acceptor by an intramolecular hydrogen bond as a fluorescence turn-on probe for cyanide. Chem Commun 2010, 46, 9197.3. C. Y. Kim, S. Park, H.-J. Kim. "Indocyanine based dual optical probe for cyanide in HEPES buffer", Dyes Pigmen. 2016, 130, 251.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-177**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly Selective Mitochondrial Cysteine Recognition by Caged Fused Oxazolidinoindole

나상윤 김해조[1,*]

한국외국어대학교 화학과 [1]한국외국어대학교 자연과학대학 화학과

We report a chromogenic and fluorescence turn-on probe based on crotonoyl ester-functionalized oxazolidinoindole for the selective detection of cysteine in neutral buffer. The probe rapidly formed indocyanophenolate through the Michael addition and a subsequent cyclization reaction of cysteine, inducing both a dramatic bathochromic shift (>130 nm) and a large fluorescence turn-on response (F/F0 12) in the UV−vis and fluorescence spectra and affording a micromolar limit of detection (LOD = 5.0 μM) of cysteine in HEPES buffer. When cysteine was added, the probe exhibited a dual optical change with strong green fluorescence and dramatic red color by the oxazolidinoindole-to-hydroxyethylindolium transformation. Further cellular application of the probe was successfully performed for the mitochondrial imaging of HeLa cells.1. Dalton, T. P.; Shertzer, H. G.; Puga, A. Annu. Rev. Pharmacol. Toxicol. 1999, 39, 67.2. Mathews, C. K.; van Holde, K. E.; Ahern, K. G. Biochemistry; Addison-Wesley Publishing Company: San Francisco, CA, 2000.3. Han, C., Yang, H., Chen, M., Su, Q., Feng, W., Li, F. ACS Appl. Mater. Interfaces, 2015, 7, 279684. Kim, C. Y., Kang, H. J., Chung, S. J., Kim, H. K., Na, S. Y., Kim, H. J. Anal. Chem. 2016, 88, 7178-7182.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-178**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Pd-Catalyzed Synthesis of Benzimidazol-2-ones

김이현 윤소원*

한양대학교 화학과

Benzimidazol-2-ones are one of the most important heterocycles found in many pharmaceuticals, and they are known to exhibit a wide range of biological activities such as inhibitions of the respiratory syncytial virus fusion, the non-nucleoside reverse transcriptase, and farnesyltransferase, the activation of K channels, and progesterone receptor antagonists. Consequently, their synthesis has received considerable attention. Herein, we present our recent result on the development of a new synthetic method for the construction of benzimidazol-2-ones through a Pd-catalyzed coupling reaction of anilines with aryl isocyanates.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-179**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-Pot Synthesis of *N*-Arylbenzimidazoles

이은미 윤소원*

한양대학교 화학과

N-Arylbenzimidazoles are a class of prominent heterocyclic motifs that play various roles in medicinal chemistry and material science. Therefore, a number of synthetic strategies have been developed for their construction. In parallel with our efforts to develop a highly efficient system for heterocyclic synthesis, we were interested in developing a one-pot synthesis of *N*-arylbenzimidazoles using readily available chemicals. Herein we report our preliminary results of the investigations into this straightforward one-pot process.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-180**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Discovery of a New Mechanistic Mode in Pd(II)-Catalyzed Oxidative Cyclization

김윤아 윤소원*

한양대학교 화학과

In general, alkylpalladium species containing a *syn* β-hydrogen atom undergoes a very well-known process, β–hydride elimination preferentially, leading to the Heck-type product. β-H elimination can be avoided when there is no *syn* β-hydrogen atom, or suppressed in the presence of various additives and ligands to facilitate the subsequent step such as reductive elimination or β-carbon elimination. Recently, we discovered a new mechanistic mode in Pd(II)-catalyzed oxidative cyclization that operates through an uncommon Pd-C bond cleavage rather than the generally preferred β-hydride elimination in alkylpalladium intermediate containing a *syn* β-hydrogen atom. In Pd(II)-catalyzed oxidative cyclization reaction of 2-alkenylphenyl 1,3-diketones, 1,2-aryl migration occurs to lead to the unexpected formation of a variety of 4-aryl-1-naphthols.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-181**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Copper-catalyzed azide alkyne cycloaddition using betaine-copper catalytic system in water

신정아 오수진 임영권*

국방과학연구소 4-2

Triazole compounds have been received wide attention by many chemists and applied to diverse fields. Since *Huisgen* reported a method of synthesis for triazoles, *Sharpless* and *Medal* proposed elegant synthetic method, copper-catalyzed azide alkyne 1,3-cycloaddition (CuAAC) to form 1,4-disubstituted-1,2,3-triazoles easily and conveniently. Recently, with respect to environmental aspects, reducing copper catalyst and organic solvent are very important issues for consideration of CuAAC. With this point of view, we developed betaine-copper catalytic system that provides easy and convenient access to the synthesis of triazoles. This catalytic system worked very efficient for affording various triazoles in water at 30^{o}C. A variety of azides and alkynes could react well to produce desired products in good to excellent yields. This system also gave easy workup, simple suction filtration or solvent extraction. Moreover, the advantages of this protocol include using the conventional copper catalytic mixture, easily generated from $CuSO_4$ and sodium ascorbate, using betaine which is easily obtained, commercially available and harmless for biological application, and no need of special designed ligands for activation and stabilization of copper catalyst. For these reasons, we believe that this efficient catalytic system can be applied broadly to biological and material fields.

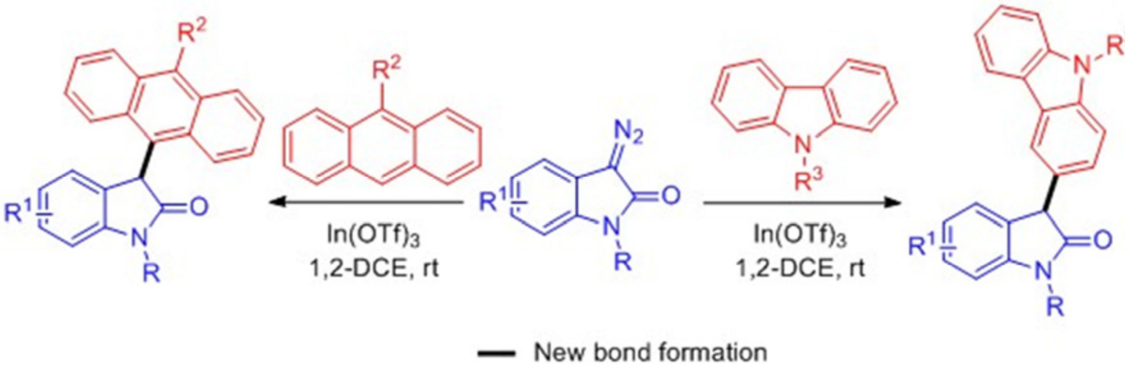
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-182**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient Approach to 3-Anthracenyloxindoles and 3-Carbazolyloxindoles *via* Indium(III)-Catalyzed Direct Arylation and Their Fluorescent Properties

소마이마가크리쉬나 이용록*

영남대학교 화학공학부

3-Substituted oxindole derivatives have dragged considerable attention of chemists because they are structural scaffold found in many natural and pharmaceutical compounds. They have shown a wide range of biological activities, such as anticancer, antibacterial and anti-inflammatory. Particularly, organic materials bearing anthracene and carbazole moieties have been studied extensively because of their significant biological activities and potential applications as functional materials in LEDs and OLEDs, semiconducting constituents in thin-film transistors, and reporters in fluorescent sensors.Due to the importance and usefulness of 3-aryloxindole derivatives, many synthetic protocols have been explored. Some of them include a reaction of aryl Grignard reagents with isatins followed by Lewis-acid promoted reductive deoxygenation, rhodium-catalyzed addition of arylboronic acid to isatins, and scandium(III)-catalyzed α-arylation of 3-substituted oxindoles with diaryliodonium salts. Other approaches have also been described, such as the palladium-catalyzed intramolecular α-arylation of amides and α-arylation reaction of oxindoles with aryl halides.To the best of our knowledge, there is no any report on the construction of 3-anthracenyloxindoles and 3-carbazolyloxindoles by Indium(III)- catalyzed arylation of 3-diazooxindoles with anthracenes or carbazoles. Herein, we describe Indium(III) triflate-catalyzed direct arylation of 3-diazooxindoles with anthracenes or carbazoles for the construction of a variety of 3-aryloxindoles bearing polyaromatic rings to develop novel functional materials and lead compounds for new drugs (Scheme 1). As application of synthetic compounds, fluorescence sensor for the detection of Hg^{2+} ions is also evaluated.


R^2
R^2
N$_2$
R^1
O
N
R
In(OTf)$_3$
1,2-DCE, rt
N
R^3
In(OTf)$_3$
1,2-DCE, rt
N
R^3
R^1
O
N
R
R^1
O
N
R
New bond formation

Scheme 1.

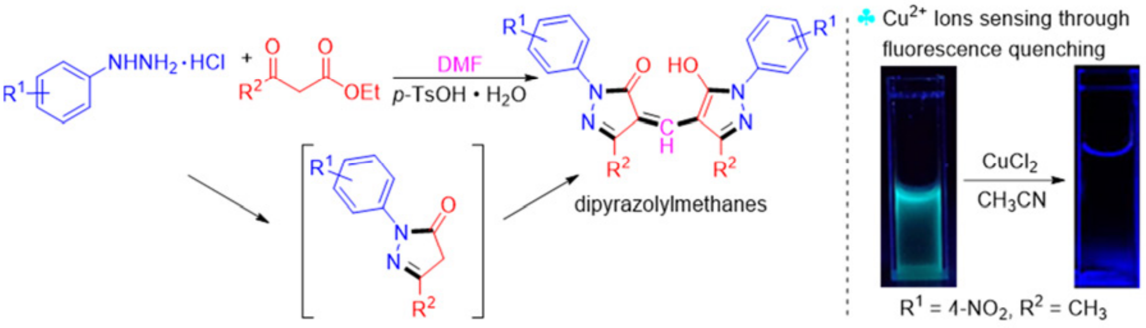
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-183**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-Pot Synthesis of Diverse Dipyrazolylmethane Derivatives and Their Application for Fluorescence Sensing of Cu^{2+} Ions

KALIAPPANKALIRAJ 이용록*

영남대학교 화학공학부

Molecules bearing a dipyrazole moiety exhibt a range of important biological activities, such as antitumor, cytotoxic, antibacterial, antifungal, anti-inflammatory, antioxidant, and molluscicidal activities. They have also been used as a building block for the synthesis of bioactive natural products and functional materials, such as ligands, UV stabilizers, and dyes. Owing to their importance and usefulness, several methods for the preparation of dipyrazole derivatives have been developed. Representative approach for the synthesis of dipyrazolylmethane derivatives includes a thermal reaction of 1-aryl-3-methylpyrazol-5-ones with quinazoline or quinoxaline. Another methods relies on the reactions of 1-aryl-3-methylpyrazol-5-ones with formamide and phosphoryl chloride ($POCl_3$) or DMSO in the presence of NaOAc and LiBr.Here, we describe an efficient synthesis of a series of dipyrazolylmethane derivatives from the reactions of readily available *β*-keto esters with arylhydrazine hydrochlorides and DMF as the carbon source and solvent in the presence of *p*-toluenesulfonic acid (*p*-TsOH). This one-pot protocol provides an easy access for structurally diverse dipyrazolylmethane derivatives. This study also provides turn-off fluorescence sensing property of the synthesized nitro-substituted compound for the detection of Cu^{2+} ions.



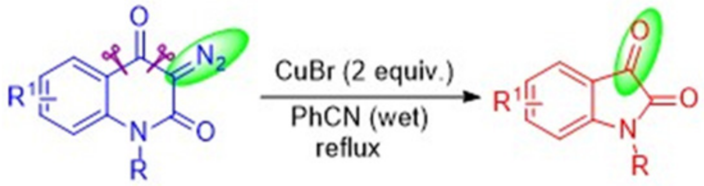
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-184**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ring Contraction of 3-Diazoquinoline-2, 4-diones: A Convenient Route Toward Diverse Isatin Derivatives

SHRESTHA RAJEEV 이용록[1,*]

영남대학교 Chemical Engineering [1]영남대학교 화학공학부

Isatins are an important class of heterocyclic compounds and have wide applications in the synthesis of biological active heterocyclic compounds. They are also known to act as anticancer, anticonvulsant, antitubercular, anti-inflammatory, antifungal, antiviral, and anti-HIV activities. Sandmeyer, Gassman, Martinet, and Stollé methods were the conventional approaches to synthesis of the isatins. Although these methods provided useful access to substituted isatins, there are noticeable drawbacks associated with relatively harsh reaction conditions, inaccessible substrates, excess amount of acid or base, multistep reactions, and limitation of substrates. Therefore, the design of general and direct strategies for the preparation of isatins, particularly involving a transition-metal-catalyzed process, would be highly interesting. Recently copper-catalyzed intramolecular C-H oxidation/acylation of formyl-*N*-arylformamides, copper-catalyzed intramolecular C-H oxidation of 2-aminoacetophenones, palladium-catalyzed double carbonylation of C-H bonds and I_2/TBHP mediated oxidation of indoles have been developed for the construction of isatins as the novel strategies. However, there is still a strong demand for a more convenient synthetic protocol for biologically interesting isatin derivatives. Herein, we present a one-pot protocol for biologically interesting isatin derivatives by copper-mediated reactions of 3-diazoquinoline-2,4-diones in wet benzonitrile (Scheme 1). The reaction proceeds *via* ring contraction through domino Wolff rearrangement, decarboxylation, bromination, substitution and dehydration. To the best of our knowledge, it is the first example of the synthesis of isatins through the decomposition of diazo compounds.


R1
O
N2
N
R
O
CuBr (2 equiv.)
PhCN (wet)
reflux
R1
O
O
N
R

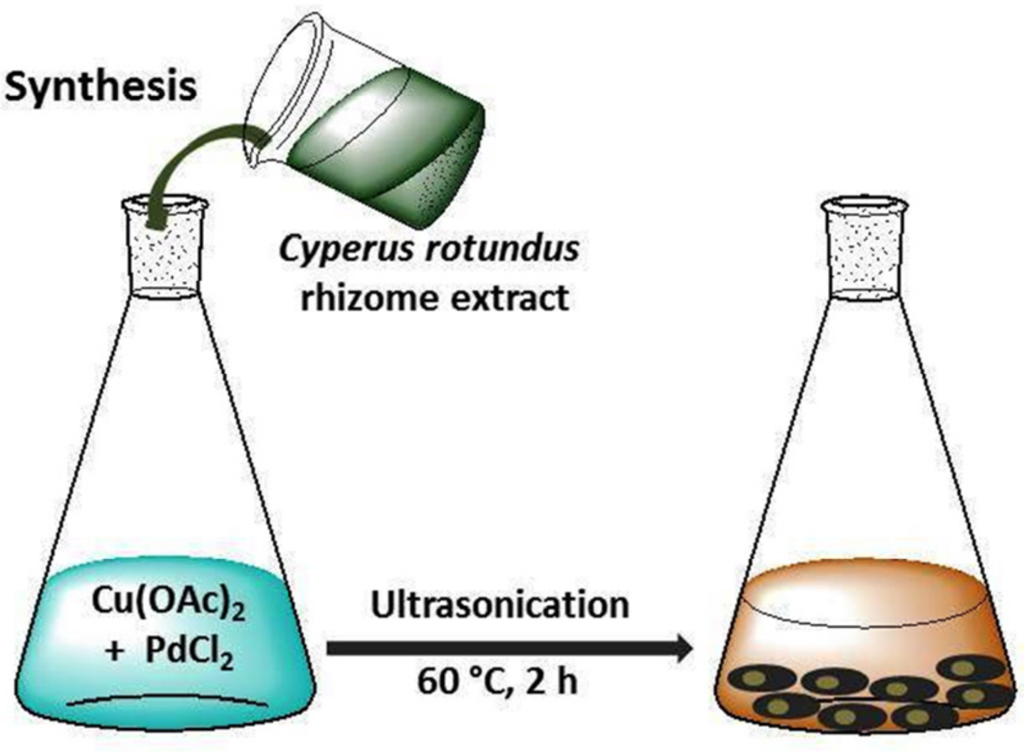
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-185**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

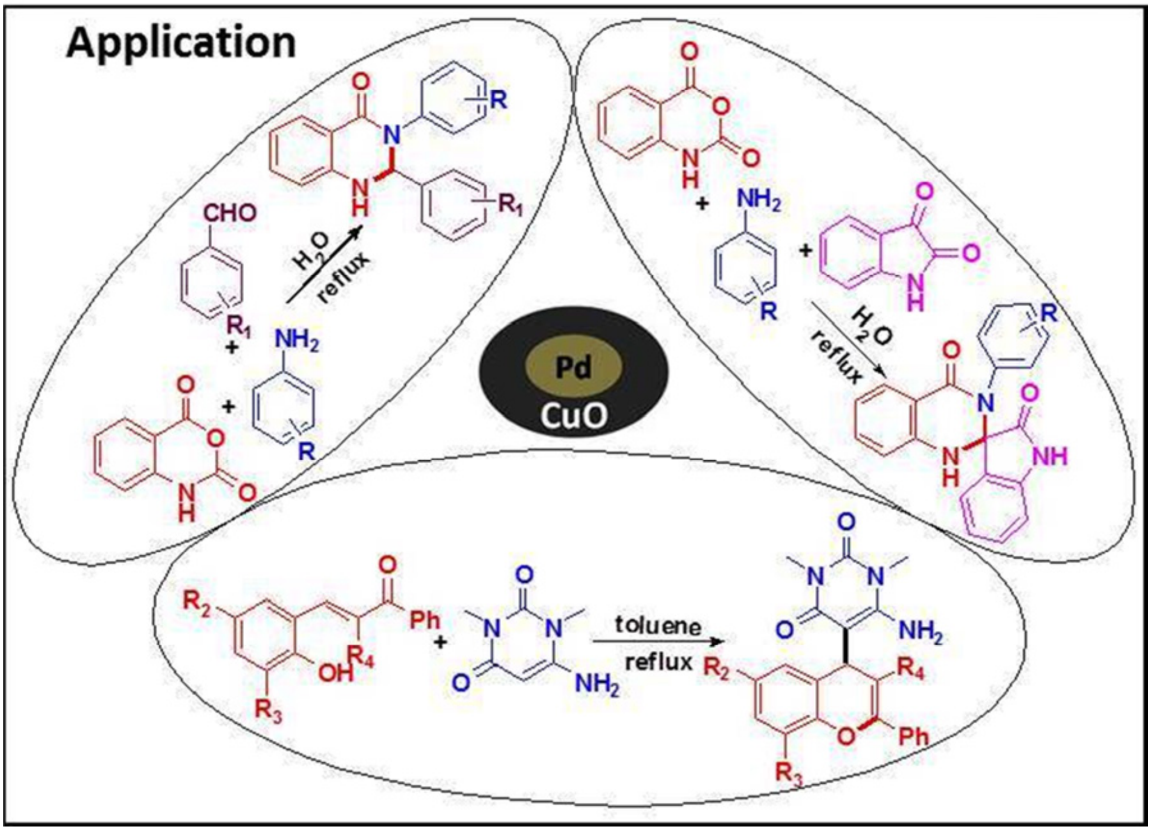
Core-Shell CuO-Pd Nanoparticles with Enhanced Catalytic Activity for the Organic Transformations

MISHRAKANCHAN 이용록*

영남대학교 화학공학부

Transition metal bimetallic nanoparticles show higher catalytic activity than their monometallic counterparts in many organic reactions. Owing to the versatile catalytic assistance of palladium, metals associated with Pd nanoparticles such as FePd, AuPd, PtPd, AgPd, and CuPd, have been used as efficient heterogeneous catalysts with excellent selectivity and activity. Many reports have emphasized the shape and size of these nanoparticles to further tune the catalytic applications. Normally, there are three different patterns of bimetallic nanoparticles; heterodimer, core–shell and nano-alloys. The core–shell pattern of nanoparticles results in superior catalytic activity to those of alloyed or heterodimers. Herein, we present a facile and green approach for the synthesis of core–shell CuO-Pd bimetallic nanoparticles using Cyperus rotundus rhizome extract as a reductant and capping agent. The synthesized nanoparticles were used as recyclable and reusable catalysts for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones, spirooxindoles, and chromenylpyrimidin-2,4-diones without significant loss of catalytic activity.


Synthesis
Cyperus rotundus rhizome extract
Cu(OAc)₂ + PdCl₂
Ultrasonication
60 °C, 2 h


Application
CHO
R₁
NH₂
R
H₂O
reflux
Pd
CuO
toluene
reflux
R₂
R₃
R₄
OH
Ph
NH₂

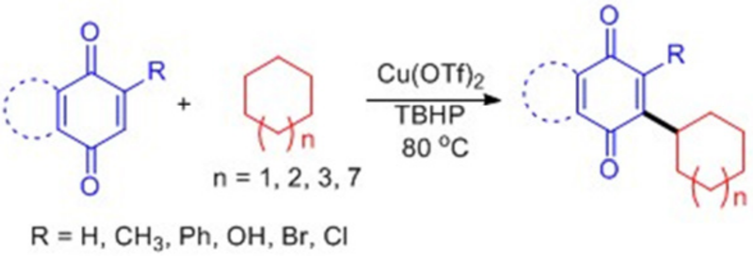
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-186**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Cross-Dehydrogenative Coupling of Quinones with Cyclic Alkanes: Rapid Access to Parvaquone and its Analogues

BARALEKRAJ 이용록*

영남대학교 화학공학부

Coupling reactions are important synthetic tools which have been widely used in organic and natural product syntheses. Due to the advantages of its atom- and step-economical nature, the direct functionalization of C-H bonds has emerged as an important cross-coupling strategy for the formation of a range of C-C bonds. This cross-dehydrogenative coupling (CDC) of C–H bonds has the merits of lower cost and environmental benignity with reduction of the number of synthetic steps. Recently, a number of methods for CDC reactions for the formation of various C-C bonds have been reported. Among these, most of reported Csp^2-Csp^3 bond formation included direct Csp^3-H bond activation adjacent to heteroatoms, carbonyl groups, and allylic and benzylic groups. Quinones have a wide range of biological properties, such as anticancer, antifungal, antibacterial, antiviral, antiprotozoal, antiplasmodial, anti-inflammatory, and trypanocidal activities. Because of their importance and usefulness, several synthetic methods for the functionalization of quinones have been developed. These methods include initial installation of a halogen on the quinones followed by palladium-catalyzed cross-coupling reactions and the direct C-H functionalization of quinones catalyzed by silver-, palladium or iron using boronic acids in the presence of co-oxidants. Here, we present the copper-catalyzed direct cross coupling reaction of quinones with cycloalkanes in the presence of TBHP (Scheme 1). This methodology allows the direct installation of cycloalkyl groups with medium and large-sized rings on the 1,4-naphthoquinones, anthracene-1,4-dione, or 1,4-benzoquinones. This protocol also provides a rapid approach for the synthesis of parvaquone as an antimalarial drug.



Scheme 1

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-187**

발표분야: 유기화학

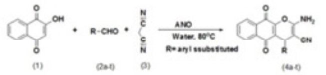
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of 4H-benzo[g]chromene-3-carbonitriles using ammonium niobium oxalate as a catalyst in aqueous media

Mudumala Veeranarayana Reddy 정연태*

부경대학교 융합디스플레이공학과

Operationally simple, green and highly efficient procedure has been developed for the diversity oriented synthesis of 4H-benzo[g]chromene-3-carbonitriles vía a domino three-component reaction utilizing various aldehydes, 2-hydroxynaphthalene-1,4-dione and malononitrile in the presence of ammonium niobium oxalate (ANO) as an eco-friendly and recyclable heterogeneous catalyst in green solvent water medium. The titled products are obtained in excellent yields in short reaction time without chromatographic separation. This green procedure proceeds easily and effectively, accommodating a variety of substituents to produce the desired products.



Scheme 1: Synthesis of 4H-benzo[g]chromene-3-carbonitrile

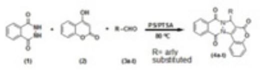
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-188**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Polystyrene-supported p-toluenesulfonic acid (PS/PTSA) -Catalyzed green synthesis of chromeno[4',3':3,4]pyrazolo[1,2-b]phthalazine-6,9,14-triones under solvent-free conditions

Mudumala Veeranarayana Reddy 정연태*

부경대학교 융합디스플레이공학과

A highly efficient, green, eco-friendly, one pot protocol has been developed for the synthesis of chromeno[4',3':3,4]pyrazolo[1,2-b]phthalazine-6,9,14-triones in excellent yields via multi-component reaction by using a catalytic amount of PS/PTSA under solvent-free condition. The merit of this protocol is less reaction time, high product yields, simple workup procedure, avoidance of toxic organic solvents, and tolerance of a wide variety of functional groups.



Scheme-1. Synthesis of chromeno[4',3':3,4]pyrazolo[1,2-b]phthalazine-6,9,14-triones

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-189**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

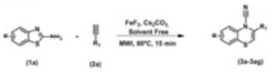
Expeditious Microwave-Assisted One-Pot Synthesis of Benzo[b][1,4]thiazine-4-carbonitrile Derivatives Catalyzed by FeF3 under Solvent-Free Conditions

Sandip Gangadhar Balwe 정연태*

부경대학교 융합디스플레이공학과

A highly efficient one pot green synthesis of benzo[b][1,4]thiazine-4-carbonitrile has been achieved under solvent-free conditions by the reaction of 2-aminobenzothiazole with terminal alkynes using microwave irradiation in the presence of Iron(III)fluoride as a catalyst. The unique features of this environmentally benign protocol are use of inexpensive catalyst, short reaction time, a wide range of functional group tolerance, easy and quick isolation of products with good to excellent yields via a simple experimental and work-up procedure. The catalyst can be recovered and reused for at least three runs without any significant impact on product yields.

Scheme


R
N
S
NH2
+
R1
FeF3, Cs2CO3
Solvent Free
MWI, 80°C, 15 min
N
R1
(1a)
(2a)
(3a-3ag)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-190**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

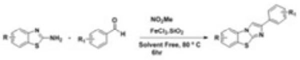
Iron(III) -Catalyzed One-Pot Synthesis of Benzo[d]imidazo[2,1-b]thiazole Derivatives under Solvent-Free Conditions

<u>Sandip Gangadhar Balwe</u> 정연태*

부경대학교 융합디스플레이공학과

An efficient, one-pot, three-component strategy for synthesis of sulfur- and nitrogen-containing benzo[d]imidazo[2,1-b]thiazole heterocycles has been developed. This cascade transformation proceeds via a transition-metal (Fe) catalyzed coupling reaction between 2-aminobenzothiazole, aldehydes, and nitromethane leading to the formation of benzo[d]imidazo[2,1-b]thiazole in good to excellent yields.

Scheme



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-191**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Characterization of Donor-Acceptor Based Small Molecules Containing Alkyne Linkage

한진희 이상경* 김성국* 강훈민 **SHAIK BAJI** 송동진

경상대학교 화학과

During recent days diketopyrrolopyrrole (DPP) based compounds have been more researched for OTFTs and organic solar cells. The diketopyrrolopyrroles have planar structure, and they have strong intermolecular hydrogen bonding and π-π stacking properties. The donor-acceptor based compounds designed and synthesized. Diketopyrrolopyrroles flanked with thiophene as an acceptors are connected with central donor groups by acetylene bonds. The synthesized compounds were characterized by NMR and mass spectroscopy. The optical properties were investigated by UV-visible absorption spectroscopy, the thermal properties were analyzed by using differential scanning calorimetry (DSC) and thermo gravimetric analysis (TGA). The electrochemical properties were analyzed by cyclic voltametry (CV). Both the compounds have shown low energy band gap. Both compounds have exhibited good thermal stability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-192**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Triazole Derivative for OLEDs Red Phosphorescence Host Materials

강훈민 이상경* 김성국* SHAIK BAJI 송동진 한진희

경상대학교 화학과

Organic light-emitting diodes (OLEDs) have advantages in full-color flat-panel displays and lighting applications. In particular, phosphorescent organic light-emitting diodes (PHOLEDs) are attractive because of their theoretical quantum efficiency can be four times higher than that of the fluorescent based OLEDs. For improving the red host PHOLEDs ability, 1,2,4-triazole derivative was designed. Synthesis and physical properties of triazole derivative for OLEDs material was reported. Triazole derivative was synthesized by well known reactions, such as Suzuki reaction, etc. Triazole derivative was confirmed by ESI-Mass, ^{1}H-NMR, ^{13}C-NMR spectroscopy and elemental analysis. The synthesized material has moderate solubility in common organic solvents such as chloroform and methylene chloride. Thermal stability was characterized by TGA and DSC. Optical and electrochemical properties of the triazole derivative was characterized by UV-vis and cyclic voltammetry (CV). The synthesized material was investigated for red host material by fabrication of electroluminescent (EL) devices. EL devices were fabricated as ITO (150 nm)/ MoO3 (2 nm)/ NPB (30 nm)/ EML[host:Ir(piq)2acac 8%] (30 nm)/ TPBi (25 nm)/ LiF (0.5 nm)/ Al(100 nm) configurations. The synthesized material based device shows 9.1 % external quantum efficiency (EQE) and 5.58 cd/A maximum power efficiency.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-193**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Liquid chromatographic resolution of proline and pipecolic acid derivates on crown-ether chiral stationary phase

조은솔 현명호*

부산대학교 화학과

Two enantiomers of a chiral compound have been known to show different biological effects on living organisms. Chromatographic resolution of the two enantiomers by high performance liquid chromatography (HPLC) has been known as one of the most accurate, convenient, and economic mean for the separation of the two enantiomers. Unlike other amino acids, it is hard for proline and pipecolic acid to be separated by using crownether CSP because they are secondary cyclic amino acids. In order to find a method to sepate proline and pipecolic acid, proline and pipecolic acid were derivatized, and separated on a chiral stationary phase (CSP) based on (+)-(18-crown-6)-2,3,11,12-tetra-carboxylic acid. In this study, the best derivatizing process and the best mobile phase condition will be provided.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-194**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Liquid chromatographic resolution of fluoxetine and its analogues on a crown ether-based chiral stationary phase

전희영 현명호*

부산대학교 화학과

Fluoxetine, known as trade name of Prozac, is an antidepressant of the selective serotonin reuptake inhibitor class. (S)-Fluoxetine is slightly more potent in the inhibition of serotonin reuptake than (R)-Fluoxetine. In this instance, the exact determination of the enantiomeric composition of fluoxetine is very important.In this study, we resolved fluoxetine and its analogues on a CSP based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid. The chiral resolution method we report here will be very valuable to the study related to the stereoselective outcome of fluoxetine and its analogues. In addition, we wish to report the structural characteristics of fluoxetine by considering the chromatographic resolution behaviors of fluoxetine analogues.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-195**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient One-pot Preparation of Asymmetrical Ureas from Cbz-protected Amines using Trifluoromethanesulfonic Anhydride

김희권

전북대학교 의학전문대학원/핵의학교실

Urea is a frequently found structure in many natural compounds and bioactive compounds such as enzyme inhibitors and antagonists. Cbz-protecting group is one of the widely used for amines due to high stability of amines during the organic synthesis. However, in order to prepare ureas from Cbz-protected amines, two separated steps including removal of the protecting group via hydrogenolysis or strong acid, and then substitution reaction were required. Herein, we report that novel practical one-pot synthetic protocol of asymmetrically substituted ureas from Cbz-protected amines using trifluoromethanesulfonic anhydride. Synthesis of asymmetrical ureas was readily performed in the treatment of 2-bromopyridine and trifluoromethanesulfonic anhydride, followed by the addition of amines. Using this one-pot synthetic protocol, various asymmetrical ureas were prepared with high yields.

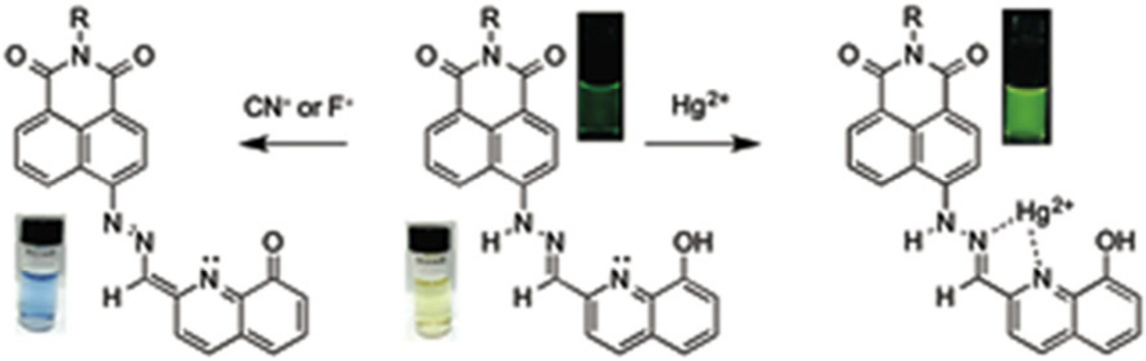
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-196**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rational design of 1,8-naphthalimide-based chemosensors for dual-mode sensing: Colorimetric and fluorometric detection of multiple analytes

나여경 홍종아 이지연[1,*]

성신여자대학교 미래응용과학과 [1]성신여자대학교 글로벌의과학과

1,8-Naphthalimide chemosensors for dual-sensing of multiple analytes were developed and tested. Sensors 1-3 contain a hydrazone linker with a bicyclic receptor group that can show chromogenic signals toward anions and fluorogenic signals toward metal ions. In particular, sensor 3 demonstrated CN- and F--specific color changes while generating Hg2+-specific fluorescence enhancement. We believe that these sensors respond to anions and cations by two distinct mechanisms, thus enabling dual-mode detection of multiple analytes.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-197**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Diversification of Imidazo[1,2-a]pyridine by microwave mediated Pd-catalyzed coupling reaction

이진희[*] 염을균[1,*]

충남대학교 자연과학대학 화학과 [1]충남대학교 화학과

Imidazo[1,2-a]pyridine derivatives exhibit interesting biological properties. It have been shown anxiolytic, antipsychotic, gastroprotective, antiimflammatory, and preventing osteoporosis.Therefore many group focus efficient synthetic methods for the heterocycles, but conventional synthetic methods showed harsh reaction condition and long reaction time. We examined microwave medicated palldium-catalyzed coupling reaction of Imidazo[1,2-a]pyridine derivatives. The synthetic method showed efficient synthetic method for diversification of heterocycles. The reaction conditions and results will be discuss.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-198**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Liquid chromatographic enantioseparation of iridium (III) complexes on HPLC chiral stationary phases

서나현 현명호*

부산대학교 화학과

Racemic iridium(III) complexes emit light with no net polarization, but enantio-enriched iridium(III) complexes emit circularly polarized light with a polarization bias. Enantio-enriched iridium(III) complexes are expected to be utilized in three dimensional electronic displays and in bioassays. In this instance, preparation of optically active iridium(III) complexes and the determination of the enantiomeric composition of optically active iridium(III) complexes are quite important. HPLC(High Performance Liquid Chromatohraphy) chiral stationary phase(CSP) method has been generally used for resolving chiral compounds, especially drugs. However resolution of enantiomers of iridium(lll) complexes on HPLC CSPs is rare.In this study, we prepared various iridium(III) complexes starting from 2-phenylpyridine and iridium chloride hydrate and resolved them on polysaccharide-based two chiral stationary phases (CSPs). Iridium(III) complexes we prepared have either a facial or meridional configuration. And each of them was separated into two enantiomers efficiently using 10% or 20% isopropyl alcohol in hexane as a mobile phase.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-199**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of novel dinuclear Ru(II) complexes containing various bridging ligands for DSSCs

이지훈 이우진 탁정애[1] 김병효*

광운대학교 화학과 [1]한양대학교 자연과학대학/화학과

Recently, Some of the researchers studied dinuclear ruthenium complexes for producing more efficient photosensitizers for DSSCs. Kumar *et al*. found that in some of case efficiency of dinuclear complex was increased 1.7 times higher than that of the structurally similar mononuclear complex. In this study, we have synthesized new heteroleptic dinuclear ruthenium(II) complexes bridged with bis-(2,2'-bipyridin-5-yl)ethyne or bis-((2,2'-bipyridin)-5-ylmethyl)amine ligands and ligated to different α-diimine ligands. Their physical and photovoltaic properties were investigated. Dye-sensitized solar cells based on some of these new dyes show reasonable efficiencies comparable with that of the standard cell based on N719.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-200**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of novel bis-pyrrole arenes from coupling reactions of nitroanilines with 1,4-diketones

배설희 김은경 이병민[1] 김병효*

광운대학교 화학과 [1]한국화학연구원 계면화학공정연구센터

Pyrroles and their derivatives have been drawn attention because of their diverse biological activities such as antibacterial, fungicidal, hypolipidemic. There are also diverse drugs containing pyrrole units such as atorvastatin, ketorolac, anti-tubulin activity and so on. Synthesis of arenes substituted with two different substituted-pyrrole moieties was investigated. Paal-Knorr condensation reaction of nitroanilines with 1,4-diketone to nitrophenyl-1*H*-pyrroles followed by indium-mediated reduction-triggered coupling reaction with another kind of 1,4-diketone resulted in two distinct pyrrole-containing arenes, *i.e.*, variously substituted 2-R-5-R'-1-((2-R-5-R'-1*H*-pyrrol-1-yl)phenyl)-1*H*-pyrroles, in reasonable yield. Sterically hindered 2,6-disubstituted nitroanilines that did show low yields were conducted by changing the reaction condition and the reaction order to overcome poor yields caused by steric hindrance.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-201**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The Synthesis of Rhodamine Hydroxamate as Acid Chemosensors

문희정 태진성*

연세대학교 화학과

The measurement of pH plays a significant role in extensive areas not only our daily life but also science and technology such as chemical and biological process control, environmental analysis, or regulation and routine monitoring in industrial process and sewage purification plants. In biological process, protons have received great attention because it is well-known that intercellular pH plays a key role in many cellular events, such as cell growth, calcium regulation, endocytosis, chemotaxis, cell adhension, and other cellular process. Lysosmoes are involved in various cell life activities, including intramolecular transportation, cell membrane recycling, and methabolism etc. The malfunction of lysosomes results in several disease about inflammation, tumors, silicosis. Therefore, in view of the significant biological function of lysosomes, it is worthwhile to design new type of probes to label lysosomes. The pH in lysosomes(pH 4.5-5.0) is more acidic than in the cytoplasm(pH 7-7.3). In this study, we have developed a pH-sensitive fluorescence sensor molecules containing rhodamine spiro 6- membered ring. The sensors have ethylene glycol groups, so we can expected that they are sensitive to acidic environment. The sensors show florescence properties in different pH rangerespectively. In addition, our probes were found to have beneficial properties for lysosome over other cell organelles. Also sensors show fluorescence intensity within zebrafish. This result seems that sensors have potential possibility for visually treating liver related diseases.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-202**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Total Synthesis of (+)-Fusarisetin A

박진영 태진성*

연세대학교 화학과

Fusarisetin A is an isolated natural product from the fungus Fusarium sp. FN080326 and expected as a valuable anticancer agent because of its biological activities. The compound potently inhibits acinar morphogenesis, cell migration, and cell invasion in MDAMB-231 cells without significant cytotoxicity. Fusarisetin A possesses an unprecedented pentacyclic ring system and acyl tetramic acid. We attempted its labotatory synthesis based on Theodorakis group and modified some reaction steps involving oxidation of alcohol, Dieckmann condensation, and aerobic oxidation of equisetin.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-203**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Light induced 1,2-Bromine Shift Reaction of alpha-Bromo Ketone

안세진 박봉서*

동국대학교 화학과

β-Halo ketones are very important precursors broad range of intermediates in organic synthesis: enones, heterocyclic derivatives, 1,3-dicarbonyl compounds, etc. Accordingly, many studies towards developing an efficient synthetic methodology of the β-halo ketones have been done in recent years. However, the methods developed so far are still unsatisfactory because of various reasons, some of which involve the use of rather exotic starting materials such as cyclopropanols or cyclopropyl ethers, which makes retrosynthetic analysis of synthetic target compounds inconvenient. It would be much better if the β-halo ketones can be obtained directly from backbone skeletons of the ketones.Several years ago, we reported that UV irradiation of α-bromo valerophenone in benzene gave β-bromo valerophenone together with valerophenone in ca. 3 to 2 ratio. In order to see how general this reaction is, we have decided to extend our research with various alpha-bromo ketones. Here we would like to report our preliminary results on the scope and variation of the reaction

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-204**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of new donor–acceptor molecule based on phenyl phenothiazine and phenyl substituted quinoline

형도성 권태우*

경성대학교 화학과

New donor-acceptor molecule that incorporate phenyl phenothiazine as the electron donor and phenyl substituted quinoline as the electron acceptor moiety have been synthesized. Phenyl phenothiazine has been used as electron donor component due to their low reversible oxidation potentials by virtue of the sulfur atom which can facilitate the hole transport of the carrier. Quinoline bromide substituted phenothiazine can play a crucial role in the synthesis of new donor-acceptor target molecules using a palladium catalyzed Stille coupling reaction with trans-1,2-Bis(tri-n-butylstannyl)ethylene. Products were determined by using ^{1}H, ^{13}C NMR, FT-IR, MS, Uv-vis and photoluminescence. Detailed synthetic routes and characterization will be described.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-205**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Isolation and characterization of new cyclic lipopeptides (surfactin isoforms) produced by Bacillus vallismortis strain BS07M

Md.Maniruzzaman Manir 문석식*

공주대학교 화학과

Bacillus vallismortis strain BS07 originally isolated from near the roots of chili pepper and has been evaluated as a potential biocontrol agent against multiple plant pathogens. In the course of characterizing bioactive compounds, we isolated three new cyclic lipopeptides, surfactin analogues including six known surfactins from the methanolic extract of solid bacterial culture broth BS07. These metabolites were purified through extraction, C-18 flash column chromatography, silica gel column chromatography, and preparative C-18 HPLC. Their structures were determined by spectroscopic method including HRTOFMS and 2D NMR and confirmed by literature data. Biological activities of these isolates are under investigation. The structures of the isolates will be presented.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

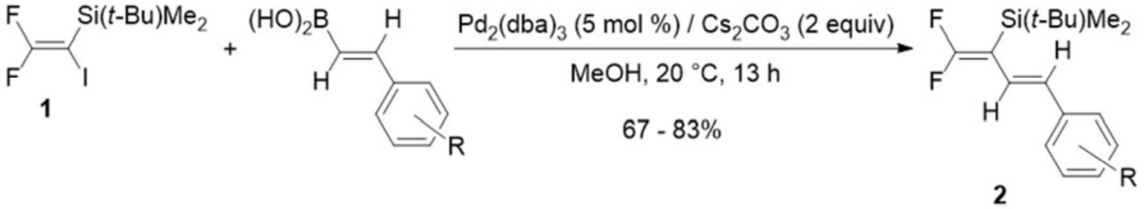
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-206**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of 2-(*t*-butyl)dimethylsilyl-1,1-difluorobuta-1,3-diene and their synthetic utility

원성용 류현규 정인화[1,*]

연세대학교 화학과 [1]연세대학교 화학및의화학과

1,1-Difluorobuta-1,3-diene derivatives are important building blocks for the synthesis of fluorinated compounds having unique biological and physical properties. 2-(*t*-Butyl)dimethylsilyl-1,1-difluoro-2-iodoethene (1), a precursor of the title compound, was prepared in high yield from the reaction of 2,2,2-trifluoroethyl iodide with 2 equive of LDA at low temperature, followed by treatment with (*t*-butyl)dimethylsilyl chloride. Suzuki-Miyaura cross-coupling reaction of 1 with various (*E*)-styrylboronic acid in the presence of $Pd_2(dba)_3$ and Cs_2CO_3 afforded the corresponding 4-aryl-2-(*t*-butyl)dimethylsilyl-1,1-difluorobuta-1,3-diene (2) in good yields. Preparation and reactions of 2 will be presented.



R = H, *p*-Me, *p*-OMe, *p*-Cl *p*-F, *p*-CF_3, *o*-Cl, *o*-OMe, *p*-Ph, etc.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-207**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Release of doxorubicin from a Gd3+-texaphyrin conjugate

이민희

숙명여자대학교 화학과

A hydrazone-based prodrug, conjugate 1, containing both doxorubicin and Gd3+ texaphyrin subunits was synthesized. The hydrazone linker in 1 undergoes acid-activated cleavage, allowing release of free Dox, a process that may be monitored by following the fluorescence enhancement at 593 nm. Confocal microscopic experiments revealed that conjugate 1 is taken up to a greater extent by A549 and CT26 cells then it is by NIH3T3 cells, which were used as a non-cancerous control. The uptake process can be monitored readily via MRI. Fluorescence-based sub-cellular localization studies provided evidence that 1 undergoes acid-activated cleavage in lysosomes. This releases free Dox, which readily translocates into the cell nuclei where it is able to promote its recognized anticancer effect. In cell proliferation experiments, conjugate 1 exhibited higher activity in the cancerous A549 and CT26 cells than in the non-cancerous NIH3T3 cells. On this basis we suggest that conjugate 1 may have a role to play as a theranostic drug delivery system that shows cancer-selective release of an active payload and which allows the fate of the conjugate and its components to be followed by two complementary imaging methods, namely Off-On fluorescence enhancement and a MR imaging.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-208**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Heterotritopic Ion Pair Receptor Based on Calix[4]pyrroles and a Bisazacrown Ether

최한별 김성국[*]

경상대학교 화학과

A new heterotritopic ion pair receptor comprised of a bisazacrown-6 and two calix[4]pyrroles was prepared for recognition of ion pairs containing divalent cations. ^{1}H NMR spectroscopic analyses confirmed that the receptor was able to bind various ion pairs including $CaCl_2$ under limited conditions. Especially, the receptor was found to form a strong complex with $CaCl_2$ where that the calcium cation was bound to the bisazacrown ether with the chloride anions being bound to the calix[4]pyrroles. Furthermore, the receptor was able to solubilize $CaCl_2$ into an organic solvent which is otherwise insoluble.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-209**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dual sensing of explosive nitro aromatic compounds by tweezer compounds

임진욱 김성국*

경상대학교 화학과

Two tweezer types of compounds were prepared as colorimetric as well as fluorometric sensors for nitro aromatic explosives. They are composed of the anthracene group as a fluorophore and two electron rich N,N-dimethylaniline groups as cooperative recognition units of electron poor explosives. In essence, they both display weak fluorescence because of PET (Photo-induced Electron Transfer) from the N,N-dimethylanilenes to the anthracene. When exposed to nitro aromatic explosives such as 2,4,6-trinitrotoluene (TNT) and 1,3,5-trinitrobenzene (TNB), they exhibited enhanced fluorescence by intercalation of TNT and TNB between two facing N,N-dimethylanilenes resulting in inhibition of the PET process. By contrast, the color changes of the receptors are attributable to the charge transfer complexation between the N,N-dimethylanilenes and the nitro aromatic compounds.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-210**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

New Indole Based-Macrocyclic Compounds and Their Anion Biding Properties

오주현 김성국*

경상대학교 화학과

New cyclo[3]amidoindole and cyclo[4]amidoindole were synthesized by stepwise EDCI coupling reactions following reduction of the nitro group and hydrolysis of the ester group of 7-nitroindole-2-carboxylate. It was found on the basis of ^{1}H NMR spectroscopic analyses that these two macrocycles are capable of binding specific anions with high selectivity depending on the ring sizes of the compounds. For instance, cyclo[3]amidoindole is selective for the chloride anion while cyclo[4]amidoindole prefers to bind a bigger anion such as the sulfate anion.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-211**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A tripodal ion pair receptor for selective recognition of lithium salts

양주호 김성국*

경상대학교 화학과

A new ion pair receptor in a tripodal shape was prepared for recognition of ion pairs containing the lithium cation. The receptor consists of three pyridine groups as cation binding sites linked via amides to three pyrrole groups for anion recognition. ^{1}H NMR spectroscopic analyses and single crystal X-ray diffraction analysis proved that this receptor is able to bind halide anions and the lithium cation highly selectively as well as lithium halide ion pairs.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-212**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

A Diazo-coupled calix[4]arene-Strapped Calix[4]pyrrole: a Colorimetric Sensor for Cesium Salts

김승현 김성국*

경상대학교 화학과

A chromogenic ion pair receptor was constructed on the basis of a diazocalix[4]arene and calix[4]pyrrole hybrid compound. In this case, the calix[4]arene subunit was locked in the conformation whereas the calix[4]pyrrole constituent are conformationally flexible. It was found by UV/vis and ^{1}H NMR spectroscopic analyses that the ion pair receptor is highly selective for cesium ion pairs. For example, upon the addition of cesium salts to the solution of the receptor, drastic color change was observed presumably as the result of formation of the cesium salt complexes by the receptor. In these ion pair complexes, the anions were bound to the calix[4]pyrrole via hydrogen bonding interactions with the pyrrolic NHs whereas the cesium cation was complexed with the oxygen atoms of the calix[4]arene and the diethylene glycol spacers. Especially, the color changes of the receptor solution is ascribable to the cesium ion bound to the oxygen atoms of the phenolic groups of the calix[4]arene linked to the diazo groups.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-213**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient Synthesis of 2,3-Dihydroisoxazole using Visible-Light Photoredox Catalysis

이중근 우상국*

울산대학교 화학과

2,3-Dihydroisoxazoles are an important class of heterocycles, widely present in many bioactive molecules. In addition to serving as drug and agrochemical targets, 2,3-dihyroisoxazoles are also valuable as synthetic building blocks in organic syntehsis. Therefore, many methods have been developed for their synthesis. The photochemical reactions of organic compounds provide a concise way to form complex molecular skeletons.We report highly efficient synthetic method for 2,3-dihydroisoxazoles using visible light photoredox catalysis (Figure 1).

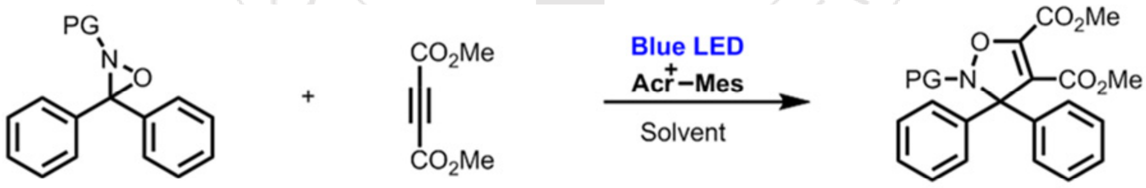


Figure 1

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-214**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

C-N bond rotation of 6-(PhO)-2,4-$(NBz_2)_2$-1,3,5-triazine and 6-(PhS)-2,4-$(NBz_2)_2$-1,3,5-triazine

이주연 김영준* 송재희[1]

충남대학교 화학과 [1]순천대학교 화학과

Thiophenol/phenol substitued dibenzylamino-1,3,5-triazines were synthesized from the reraction of cyanuric chloride and thiophenol/phenol followed by the reaction of dibenzylamine.We obtained the activation energy of C-N bond rotation of the compounds from the variable temperature NMR experiments in DMSO-d_6 and Toluene-d_8.And the free energy of coalescence (ΔG_C‡) for C-N bond rotation in the thiophenol and phenol substitued dibenzylamine-1,3,5-triazines was measured from not only coalescence temperature but also line shape analysisThe energy of activation in DMSO-d_6 was slightly greater than in Toluene-d_8.The results were compared with the activation energy of C-N bond rotation of other substitued dibenzylamino-1,3,5-triazines.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-215**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Visible-light photoredox-catalyzed alkylation/ring expansion sequences of 1-(1-arylvinyl)cyclobutanol derivatives

김연주 권수진 김대영*

순천향대학교 화학과

A visible-light-mediated photocatalytic bis(alkoxycarbonyl)methylation/ ring expansion of alkenyl cyclobutanols is described. This approach provides a mild and operationally simpleaccess to the synthesis of bis(alkoxycarbonyl)methyl-substituted cyclic ketones from the coupling reaction of 1-(1-arylvinyl)cyclobutanols with alkyl bromomalonates.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-216**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Visible-light photocatalyzed arylation/semi-pinacol rearrangement cascade of allylic alcohols

권수진 김대영*

순천향대학교 화학과

A visible-light-mediated photocatalytic arylation/1,2-carbon migration of alkenols is described. This approach provides a mild and operationally simple access to the synthesis of aryl-substituted cyclic ketones via arylation and 1,2-carbon migration of 1-(1-arylvinyl)cyclobutanol derivatives.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-217**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enantioselective addition of diphenyl phosphonate to ketimines derived from isatins catalyzed by binaphthyl-modified organocatalysts

김유빈 김대영*

순천향대학교 화학과

Chiral binaphthyl-modified squaramide-catalyzed enantioselective addition of diphenyl phosphonate to ketimines derived from isatins has been achieved. This method affords practical and efficient access to chiral 3-amino-3-phosphonyl-substituted oxindole derivatives in high yields with excellent enantioselectivities (up to 99% ee).

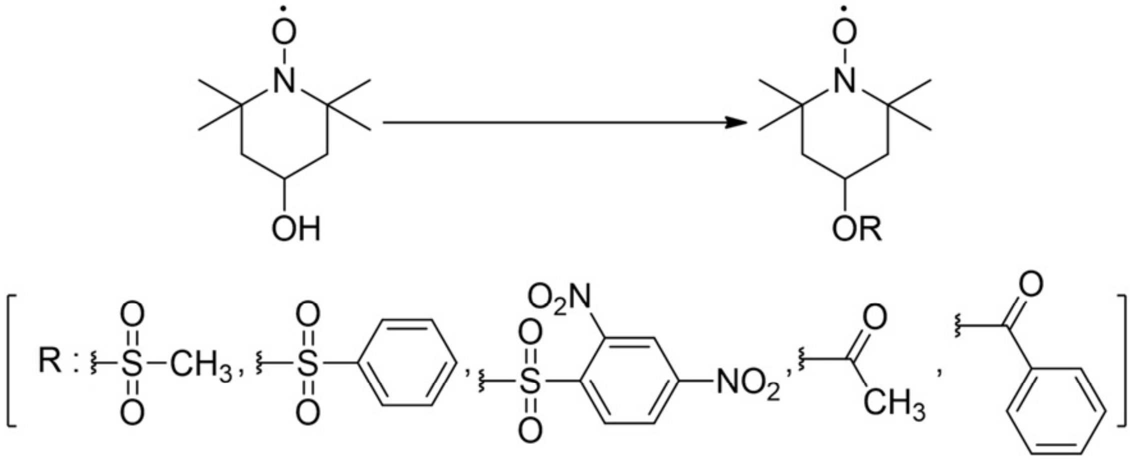
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-218**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation and Electrochemical Investigation of TEMPOL Derivatives: Apply to Redox Flow Battery

성현준 안철진*

창원대학교 화학과

Recently TEMPOL derivatives are interesting to 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 derivatives. To do this we prepared TEMPOL derivatives and investigated CV results depending on their different functional group.



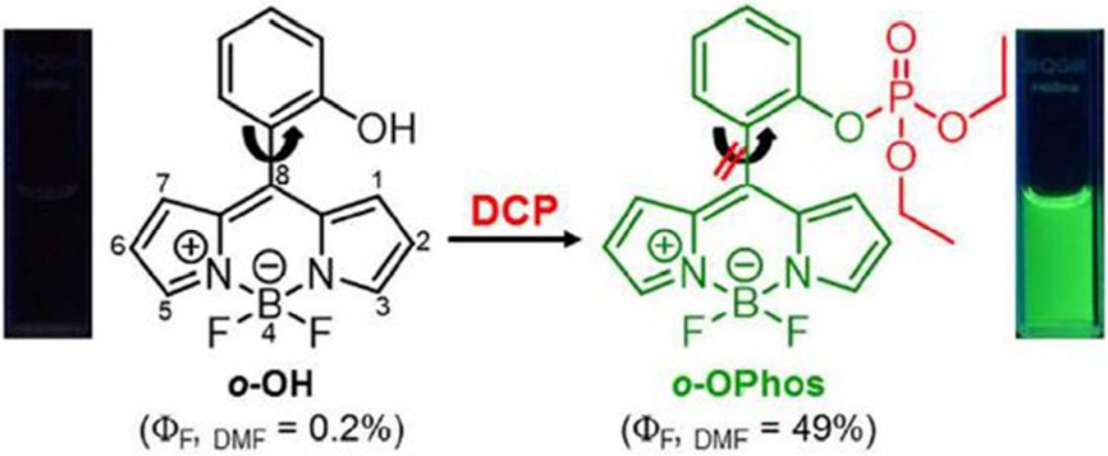
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-219**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Molecular Rotors for the Detection of Chemical Warfare Agent Simulants

김태일 김영미[1,*]

경희대학교 화학과 유기화학전공 [1]경희대학교 화학과

Organophosphorus (OP) nerve agents, including sarin, soman, and tabun (Figure a), are extremely toxic volatile liquids that block the function of acetylcholinesterase, a key enzyme in neurotransmission, leading to convulsions and ultimately death by respiratory paralysis. Accordingly, it is highly important to develop efficient methods for the monitoring of level of nerve agents in threat situation. In this presentation, we reported the BODIPY-based fluorescence turn-on probe *o*-OH, which is designed based on the modulation of molecular rotor system, for the sensitive and selective detection of nerve agent simulants. In DMF, *o*-OH has a low fluorescence quantum yield (φ_F = 0.002) and a short excited-state lifetime (τ_{av} = 0.11 ns) due to free rotation of meso C–Ar bond. But, upon the addition of diethyl chlorophosphate (DCP), which is used as a simulant of nerve agents, the reaction of *o*-OH with DCP forms strong emissive phosphorylated product *o*-OPhos. (Figure b) *o*-OPhos has remarkably high quantum yield (φ_F = 0.49) and relatively long excited-state lifetime (τ_{av} = 4.39 ns), possibly due to the restriction of free rotation by bulky phosphoryl group. Notably, the fluorescence response of *o*-OH to DCP at low concentrations (0–3 mg/L) showed linear relationship, resulting in considerably low limit of detection for DCP (0.71 μg/L). *o*-OH not only showed high selectivity in the presence of various analytes but also successively performed solid-state device test in order to evaluate feasibility under a real threat situation. Subsequently, sensitivity and selectivity of *o*-OH to DCP make it suitable for the development of practical low-cost paper strips against OP CWA threats.


OH
8
7
1
6
2
5
3
4
N
B
F
DCP
O
P
o-OH
($\Phi_{F,\ DMF}$ = 0.2%)
o-OPhos
($\Phi_{F,\ DMF}$ = 49%)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-220**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Pyrimidine-based donor-acceptor copolymers semiconductor for controlling organic solar cell performance

구다솜 서홍석*

부산대학교 화학과

Organic solar cells (OSCs) have been recognized as a one of the most powerful renewable energy. To improve efficiency of organic solar cells, we designed and synthesized the pyrimidine-based copolymers, PBDTF, PBDTTCN, PBDTCN and PBDTTF, by using 4,8-bis(5-(2-octyldodecyloxy)thiophen-2-yl)benzo[1,2-*b*:4,5-*b*0]dithiophene (BDTT) or 4,8-bis(2-octyldodecyloxy)benzo[1,2-*b*;3,4-*b*0]dithiophene (BDT). The device using PBDTF and $PC_{71}BM$(1:1.5) with DIO showed a V_{OC} of 0.64 V, a J_{SC} of 2.26 mA/cm^2, and a fill factor (*FF*) of 0.35, giving a power conversion efficiency of 0.50%. The device using PBDTTCN and $PC_{71}BM$(1:1.5) with DIO showed a V_{OC} of 0.86 V, a J_{SC} of 3.14 mA/cm^2, and a *FF* of 0.40, giving a power conversion efficiency of 1.09%. The device using PBDTCN and $PC_{71}BM$(1:1.5) with DIO showed a V_{OC} of 0.74 V, a J_{SC} of 2.37 mA/cm^2, and a *FF* of 0.36, giving a power conversion efficiency of 0.63%. The device using PBDTTF and $PC_{71}BM$(1:1.5) with DIO showed a V_{OC} of 0.82 V, a J_{SC} of 3.28 mA/cm^2, and a *FF* of 0.39, giving a power conversion efficiency of 1.05%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-221**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Syntheses of conjugated polymer with indenoindene for organic photovoltaic devices

김민지 서홍석*

부산대학교 화학과

We synthesized the novel conjugated polymers with dihydroindeno[2,1-*a*]indene moiety (ININE), very planar electron-pushing group, for the organic photovoltaic devices (OPVs) . The D-A conjugated polymers, both of P1 and P2 have a electron pulling group of *N*-alkyl-2,2′-bithiophene-3,3′-dicarboximide (BTI) and electron pushing group of ININE for the more extensive UV absorption region. Absorption peaks of P2, fused thiophene unit liking the electron pulling and pushing groups, was shifted to the bathochromic wavelength range than P1. The synthesized P1, P2 polymers indicated deep energy levels of HOMO at -5.76 and -5.59 eV respectively and energy levels of LUMO at -3.65 and -3.55 eV respectively. The device containing P2 and $PC_{71}BM$ (1:2) with DPE indicated a V_{OC} of 0.80 V, a J_{SC} of 1.59 mA/cm^2, a fill factor (*FF*) of 0.39 and a power conversion efficiency of 0.49%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-222**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Amphiphilic Homopolymers and Their Self-Assembly into Acid-Responsive Polymeric Micelles

손창국 양시경*

전남대학교 화학교육과

We present a strategy for preparing amphiphilic homopolymers as building blocks for self-assembly into supramolecular nanostructures. The synthesis begins with norbornene monomers containing oligoethylene glycols on the side-chains. Ring-opening metathesis polymerization (ROMP) of the monomers and subsequent dihydroxylation afford water-soluble, dihydroxylated poly(norbornene)s (PNBs). Amphiphilic modifications of the hydrophilic PNBs can be achieved by reacting 1,2-diols on the backbones with hydrophobic dodecanals to form acetal linkages. The self-assembly of the resulting amphiphilic PNB homopolymers affords polymeric micelles whose morphologies can be tuned by breaking the acetal linkages under acidic conditions, as shown in the scanning electron microscopy (SEM) images.

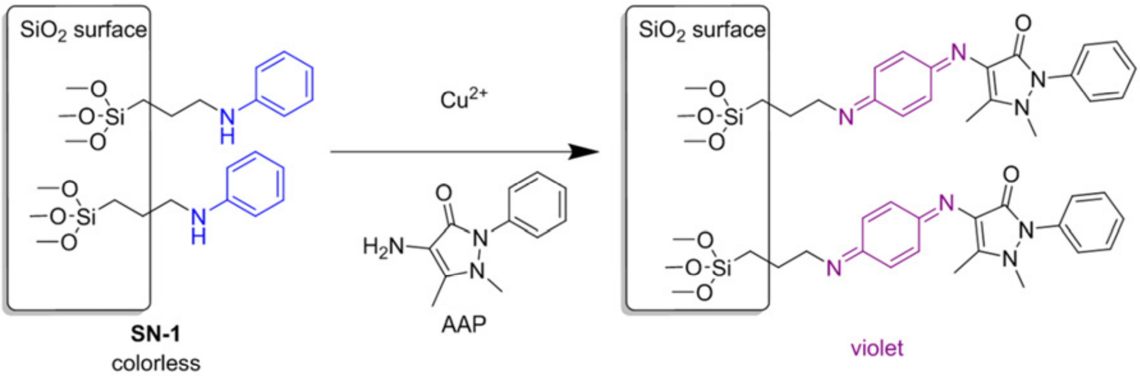
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-223**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Colorimetric determination of Cu^{2+} ions using silica nanoparticles via formation quinonediimine dye

김다빈 장석규*

중앙대학교 화학과

In this study, we report a new Cu^{2+}-selective signaling system using the Cu^{2+}-assisted oxidative coupling of aniline with 4-aminoantipyrine (AAP) to form chromogenic quinonediimine dye. Because anilines are toxic substances, we immobilize anilines in a suitable support to make aniline-functionalized silica support, **SN-1**. The designed system provides a prominent colorimetric signaling behavior toward Cu^{2+} ions by color change from colorless to violet. The Cu^{2+}-induced color change was naked-eye detectable and completed within 3 minutes after sample preparation, which confirmed the high-speed response of the **SN-1**. The Cu^{2+}-selective signaling system was not affected in the presence representative metal ions as a background. In addition, detection limit was estimated to be 1.98×10^{-6} M (0.13 ppm) in aqueous environments. As a practical application, convenient detection of Cu^{2+} ions using an electronic device as an easily available signaling capture tool was conducted.



SN-1
colorless

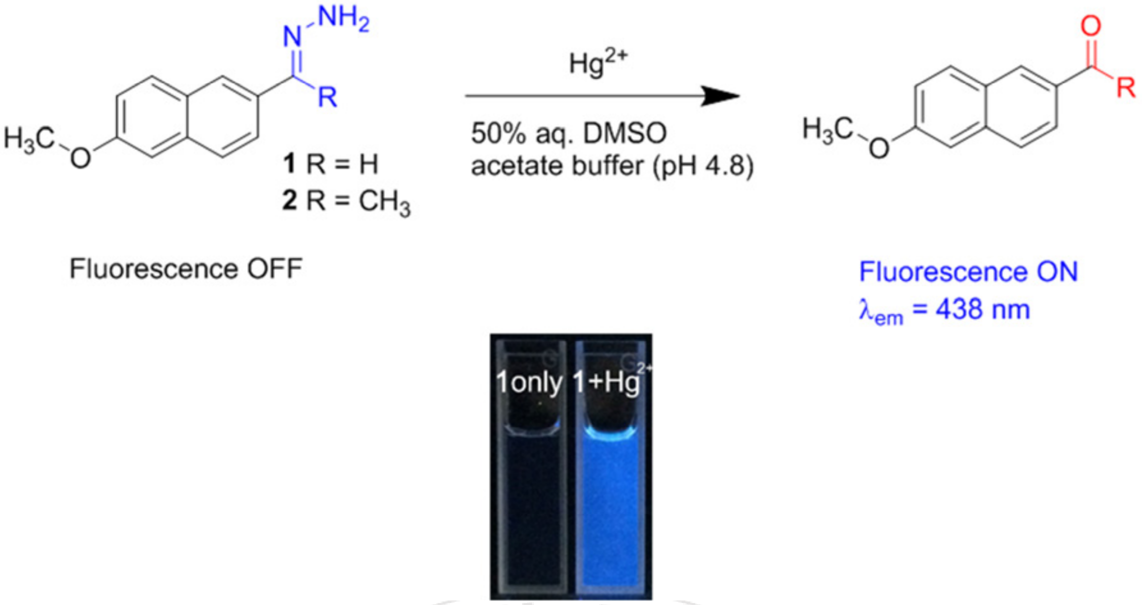
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-224**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Hg^{2+}-selective fluorogenic signaling probe based on the hydrolysis of hydrazone

류혜인 장석규*

중앙대학교 화학과

Simple Hg^{2+}-selective fluorescent signaling probes based on methoxynaphthalene hydrazone were investigated. To design more effective probe, aldehyde- and ketone-based hydrazone derivatives were synthesized and both probes showed fluorogenic signaling toward Hg^{2+} ions. However the aldehyde-based hydrazone **1** exhibited much faster fluorescent enhancement than the ketone-based hydrazone **2** did in response to Hg^{2+} ions in a 1:1 mixture of acetate buffer (pH 4.8) and DMSO. The fluorescence increase was due to the Hg^{2+}-selective hydrolysis of hydrazone to afford the strongly fluorescent methoxynaphthaldehyde. The transformation from hydrazone to aldehyde was verified by changes of proton peaks in ^{1}H-NMR and comparison of spots on TLC plate. Hg^{2+}-selective signaling of **1** was not affected by the presence of representative metal ions as background. In addition Hg^{2+}-selective fluorescence signaling by **1** was possible with a detection limit of 6.0×10^{-6} M. As a practical application, convenient detection of Hg^{2+} ions using a smartphone as a portable signaling processor was conducted.


H3C
O
N
NH2
R
1 R = H
2 R = CH3
Fluorescence OFF
Hg2+
50% aq. DMSO
acetate buffer (pH 4.8)
H3C
O
O
R
Fluorescence ON
λem = 438 nm
1only
1+Hg2+

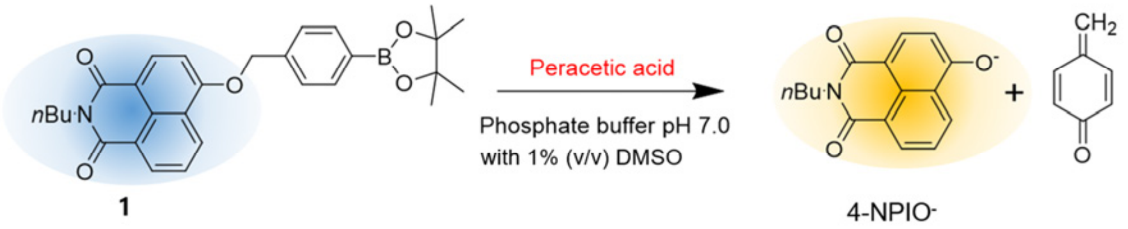
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-225**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A new peracetic acid-selective signaling probe based on oxidative cleavage of a naphthylimide-boronate

황금샘 장석규*

중앙대학교 화학과

A new peracetic acid (PAA)-selective signaling probe 1 based on oxidative cleavage of naphthylimide-boronate pinacol ester was developed. Probe 1 exhibited selective signaling behavior towards PAA over other commonly used practical oxidants such as H_2O_2 and HOCl. The PAA signaling was due to the oxidative cleavage of boronate moiety of 1 to form strongly fluorescent 4-hydroxynaphthalimide (4-NPIOH). The PAA signaling was not affected by the presence of common metal ions and representative anions. As a practical application, signaling of 1 for determination of PAA levels in practical samples was conducted by using an easy-to-use smartphone as a detection tool.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-226**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Design of conjugated polymers based on pyrimidine derivatives and applications in solar cells

김민지 서홍석*

부산대학교 화학과

Organic photovoltaics (OPVs) have been deeper developed due to their advanced properties including low cost, light-weight, mechanical flexibility, easy processability and large-scale production.1-2 We synthesized conjugated polymers based on PTTICN, PTTICNR and PTTIFR, including TTI, 2-fluoropyrimidine and 2-pyriminecarbonitrile. It was applied to evaluate the properties of the conjugated polymers. The optical band gaps from UV-vis absorption onset of PTTICN, PTTICNR and PTTIFR were about 2.0 eV. The HOMO energy levels of polymers (PTTICN, PTTICNR and PTTIFR) were at -5.26 ~ -5.34 eV, their LUMO energy levels were at -3.47 ~ -3.50 eV, and the electrochemical band gap of around 1.8 eV. The device including PTTICN and $PC_{71}BM$ (1:4) with DIO indicated a V_{OC} of 0.82 V, a J_{SC} of 6.38 mA/cm^2, and a fill factor (*FF*) of 0.54, giving a power conversion efficiency of 2.81%. The device of PTTICNR and $PC_{71}BM$ (1:4) with DIO showed a V_{OC} of 0.81 V, a J_{SC} of 6.38 mA/cm^2, and a *FF* of 0.43, giving a power conversion efficiency of 2.22%. The device comprising PTTIF and $PC_{71}BM$ (1:4) with DIO showed a V_{OC} of 0.64 V, a J_{SC} of 7.38 mA/cm^2, and a *FF* of 0.55, giving a power conversion efficiency of 2.61%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-227**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole based conjugated polymers and application for organic solar cells

구다솜 서홍석*

부산대학교 화학과

Organic solar cells (OSCs) have interested as advantages of low cost, large area, light weight and large scale solution processing. We designed and synthesized new conjugated polymers, PTTIBT and PTTIMBI, including 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole. After the polymers applied to OSCs, we investigated the photovoltaic characteristics. The optical band gaps from UV-Vis absorption onset of PTTIBT and PTTIMBI were 1.68 eV and 1.54 eV, respectively. The HOMO energy levels of two polymers were at -5.32 eV and -5.29 eV, their LUMO energy levels were at -3.50 eV and -3.61 eV. The device comprising PTTIBT and $PC_{71}BM$ (1:1.5) with DIO showed a V_{OC} of 0.62 V, a J_{SC} of 3.28 mA/cm^2, and a fill factor (*FF*) of 0.42, giving a power conversion efficiency of 0.85%. The device comprising PTTIMBI and $PC_{71}BM$ (1:1.5) with DIO showed a V_{OC} of 0.69 V, a J_{SC} of 7.10 mA/cm^2, and a *FF* of 0.53, giving a power conversion efficiency of 2.60%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-228**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Polyphenolic components from *Thymus schimperi* Ronninger: LC-ESI-MS/MS characterization and quantification

DestaKebedeTaye

경상대학교 화학과

Thymus schimperi is a plant known for its medicinal use in many parts of the world including East Africa. People in Ethiopia, where the plant is widely distributed, use it as tea for treatments of various health ailments such as cold and fever. Previous studies on the plant majorly focus on the characterization of essential oils. Here, in this study, LC-ESI-MS/MS method was used for characterization of polyphenolic components from *T. schimperi* sample collected from Ethiopia. A 1100 series HPLC system (Agilent Technologies, Santa Clara, USA) and a hybrid triple quadrupole/linear ion trap 3200 Q TRAP mass spectrometer (Sciex LLC, Framingham, USA) were used. A gradient elution starting with 10% B followed by an increase to 40% for 40 min, to 55% for 5 min, to 70% for 10 to 75% for 5 min and an isocratic elution for the last 5 min using a binary solvent system (0.1% acetic acid (solvent A); and 0.1 % formic acid in 1:1 ratio of MeOH and ACN (solvent B) was applied throughout the analysis. Structural characterization of the polyphenols was achieved from $[M-H]^-$ and/or $[M+H]^+$ ion peaks and MS/MS fragment ions along with extensive literature data. The identified molecules were quantified using standard flavonoids having similar chromophore and the method was validated. Anti-inflammatory activity tests of the total extract is underway.

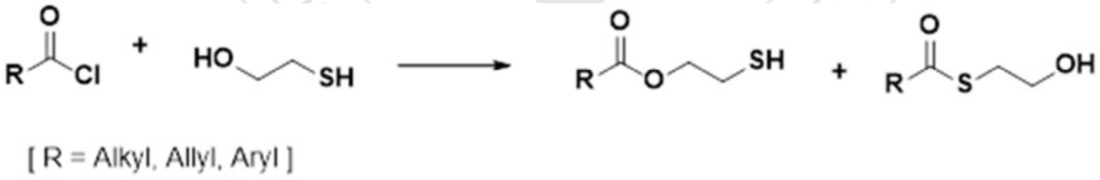
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-229**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The Investigation of Chemoselectivity in β-mercaptoethanol with Acid Chloride Derivatives

정완희 안철진*

창원대학교 화학과

The functionalized molecules bearing free –SH are considered important to prepare the encapsulated gold nanoparticles with functionalized group and protect against radiation-induced damage to DNA. The selective O- or S- acylation of mercatoalcohols are synthetically important to prepare functionalized molecules bearing free –SH. In this poster, we want to present convenient and simple procedure for chemoselective O-acylation of mercaptoethanol and mercatophenol with acid chloride derivatives. To support our results, the kinetic and thermodynamic data will be discussed too.



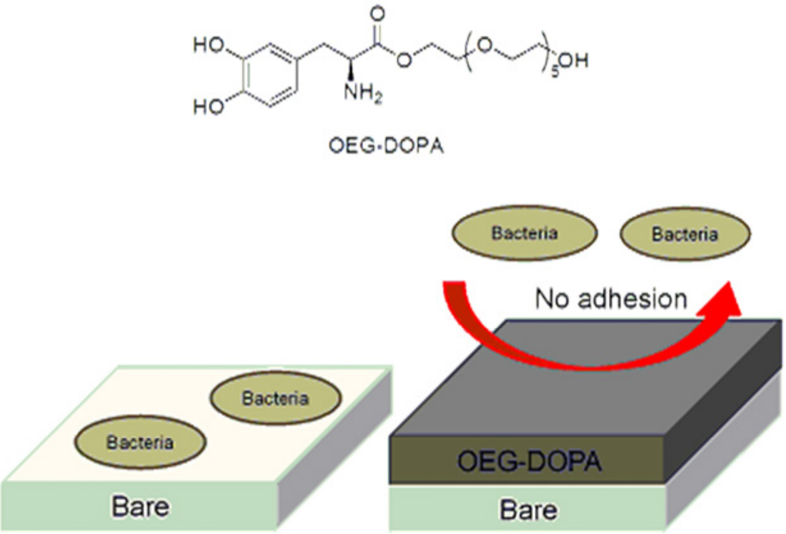
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-230**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of a Non-biofouling Dopamine Derivative and its Antibacterial Application

기소현 이슬기[1] 송수정[1] 조우경[*] 최준식[1]

충남대학교 화학과 [1]충남대학교 생화학과

Bacteria can adhere to a surface using adhesive proteins and they rapidly proliferate, forming three-dimensional community named as biofilm. Biofilm can cause severe medical infection and can be crucial problems for the implantable medical devices. The surface modification with non-biofouling materials has been recognized as one of efficient approaches to suppress the formation of bacterial biofilm. Ethylene glycol/zwitterion-based materials have been used for the purpose, however, there is still unmet need to develop a facile and universal coating material for preventing bacterial adhesion on any kind of surface. Inspired by mussel's adhesive proteins, we synthesized a dopamine derivative via esterification of oligo(ethylene glycol) (OEG) with *L*-3,4-dihydroxyphenylalanine (*L*-DOPA). It is designed to have catechol and amine moieties for one-step, facile coating without any additives (e.g., polydopamine adlayer). *L*-DOPA was used to mimic the catechol-containing mussel adhesive proteins. Titanium dioxide (TiO_2), which has been widely used as a medical material, was coated with the dopamine derivative (OEG-DOPA). OEG-DOPA-coated substrates were characterized by ellipsometry, contact angle goniometry, FT-IR, X-ray photoelectron spectroscopy, and atomic force microscopy. The bacterial adhesion was investigated with gram-negative *E.coli* and minimal bacterial adhesion was optimized in this study.


HO
HO
O
O
O
5
OH
NH2
OEG-DOPA
Bacteria
Bacteria
No adhesion
Bacteria
Bacteria
OEG-DOPA
Bare
Bare

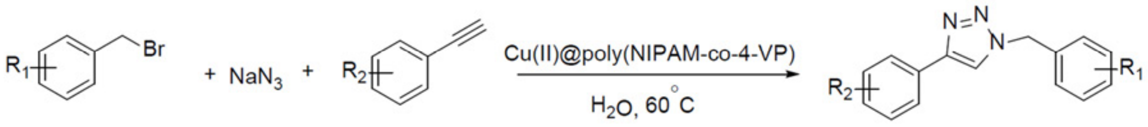
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-231**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of 1,2,3-Triazoles Catalyzed over Copper Supported on a Thermoresponsive Polymer in Water

임민경 이경미[1] 고성현[1] 이학준[*]

한양대학교 응용화학과 [1]한양대학교 바이오나노학과

Poly(NIPAM-co-4-VP), synthesized from *N*i-isopropylacrylamide and 4-vinylpyridine with a 1:1 monomer ratio, exhibits a temperature-dependent phase transition in water. In this study, we synthesized the heterogeneous polymeric catalyst by immobilization of copper sulfate in a Poly(NIPAM-co-4-VP). A series of 1,4-disubstituted-1,2,3-triazoles were synthesized regioselectively in water by the one-pot reaction. This catalyst can be reused for several times.



R_1= H,CH_3,OCH_3,Br,Cl, NH_2,CF_3···
R_2= H,CH_3,OCH_3,NO_2,Cl...

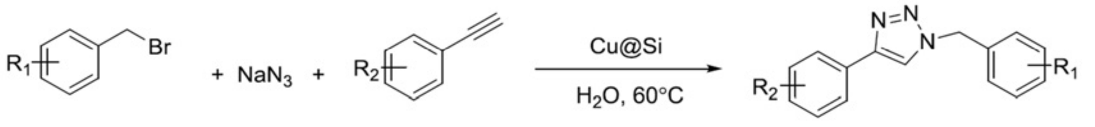
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-232**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Click Chemistry in Aqueous Media Using Immobilized Cu Catalyst

이희진 반재영 정유리 이학준[1],*

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

The click chemistry is the Copper-catalyzed reaction of an azide with an alkyne to form a 5-membered heteroatom ring: azide-alkyne cycloaddition. We have investigated the one-pot click chemistry using Cu catalyst. 2-Pyridinecarboxaldehyde ligand was anchored on commercially available 3-aminopropyl-functionalized silica gel followed by Cu metal immobilization. The 1,4-substituted triazole compounds were isolated after work up in a good yield. Results showed that silica immobilized catalyst could be recycled over several times without considerable loss on its activity.



R_1= H,CH_3,OCH_3,Br,Cl, NH_2,CF_3...
R_2= H,CH_3,OCH_3,NO_2,Cl...

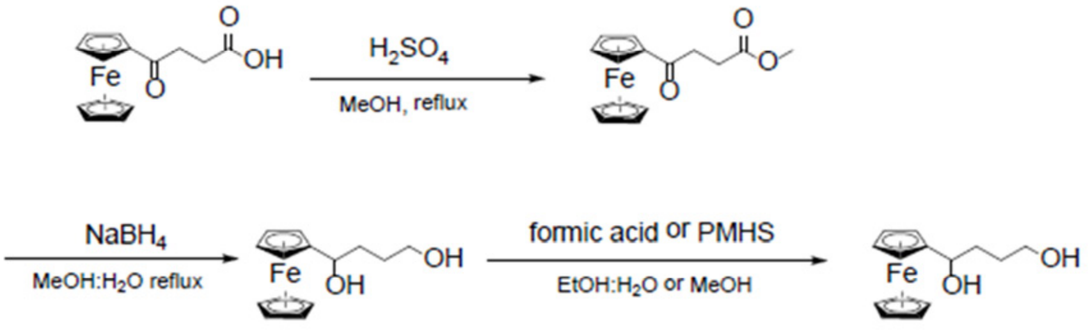
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-233**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

An efficient synthesis of ferrocene derivative as a rocket propellant oxidizer

김한철 이희진 이학준[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

Ferrocene compound is used as a combustion catalyst of rocket propellants. However, the compound is not homogeneously mixed with the propellants. To solve this problem, various Ferrocene derivatives have been used. 4-Ferrocenyl butanol is one of the ferrocene derivatives. Current synthetic methods for 4-Ferrocenyl butanol are using lithium aluminum hydride, which is extremely violent and dangerous. Herein, we found a new synthetic method avoiding lithium aluminum hydride, which will be able to apply on a development of manufacturing process.



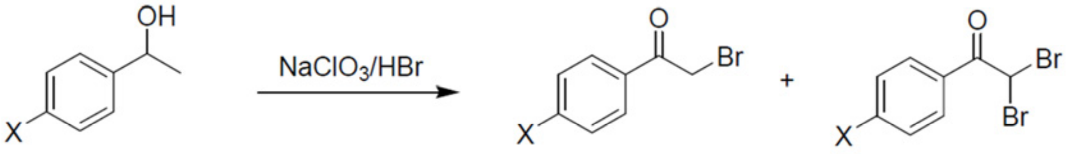
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-234**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

In Situ-Generated Bromine by HBr-$NaClO_3$One-pot Oxidation and α-Bromination of Benzyl Alcohol in Water

고성현 이학준[1,*] 정유리

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

α-Bromination has been widely employed in organic synthesis for key reaction intermediates not only their own impact and identity but they are also precursors of various biologically and industrially important compounds. Most of the brominating reagents require careful handling and toxic by-products. Herein, we report the a green process for one-pot oxidation and α-bromination in situ-generated bromine from $NaClO_3$ with hydrobromic acid that helps in the synthesis of α-bromoaryl ketones from benzyl alcohol under mild conditions using water as solvent.



X =-H, OH, OCH_3, CH_3, NO_2, CN, Cl, Br, $COOCH_3$

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-235**

발표분야: 유기화학

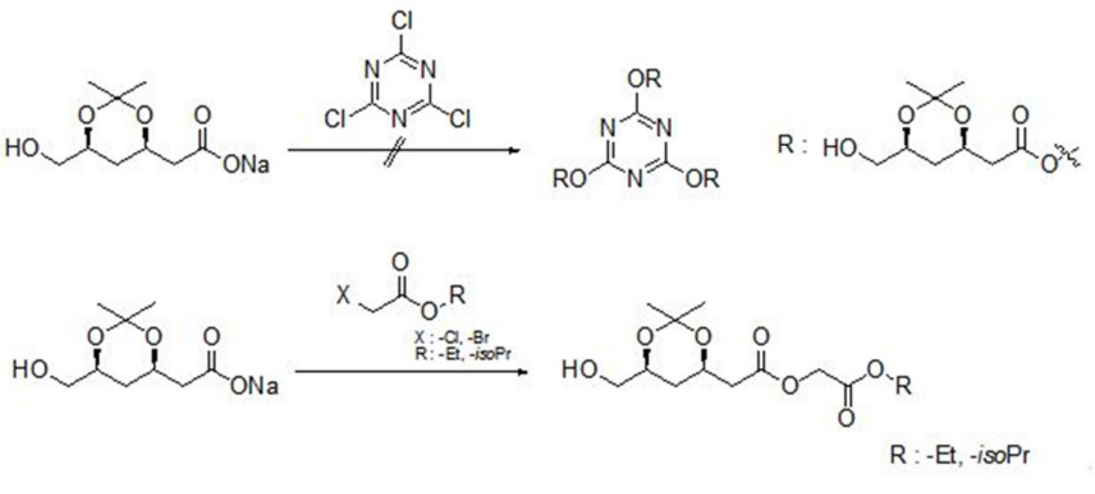
발표종류: 포스터, 발표일시: 금 11:00~12:30

A new synthetic process for the Rosuvastatin intermediates

반재영 정유리 이학준[1,*]

한양대학교 바이오나노학과 [1]한양대학교 응용화학과

According to westernized eating habits, hyperlipidemia incidence rate has been increasing in Korea. Due to the fact, the demand for therapeutic agents for hyperlipidemia has been also increasing. Among the various agents, Rosuvastatin is more biocompatible and has less side effects. Herein, the synthetic strategy to avoid present patents, we found a different protecting group to afford a new synthetic process of Rosuvastatin intermediates. The below reaction scheme represented our trials for the synthesis of the intermediates.



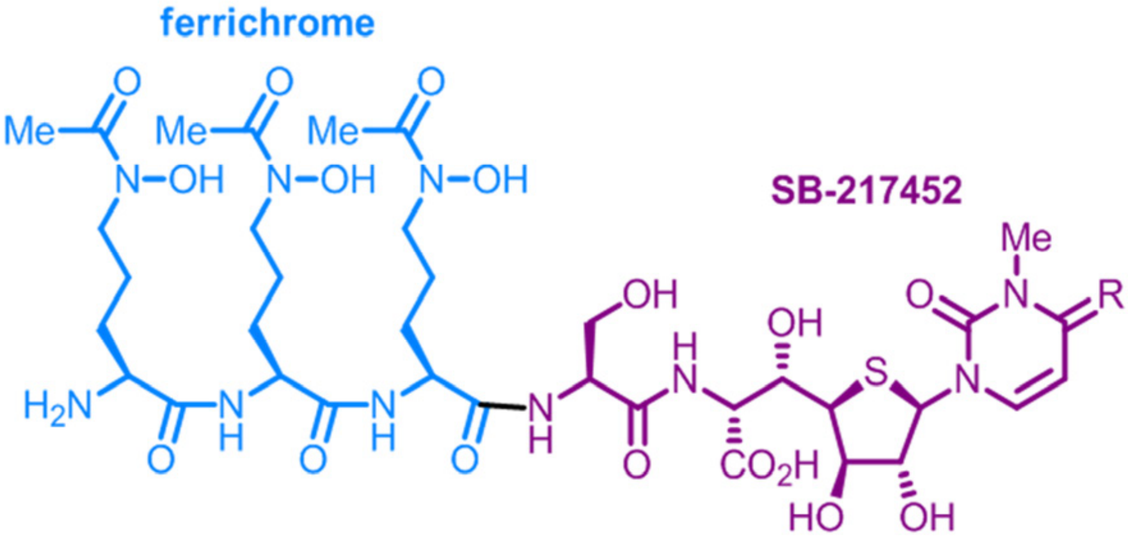
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-236**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Studies toward chemoenzymatic synthesis of SB-217452, a thionucleoside core of albomycin δ_2

박예송 황진효 송운영 김학중*

고려대학교 화학과

Albomycins are naturally occurring sideromycins produced by some streptomycetes. They are Trojan horse antibiotics consisting of a modified seryl thionucleoside compound, SB-217452, and a ferrichrome-like siderophore. Mechanistically, the nucleoside portion of albomycins were found to act as an inhibitor of bacterial seryl-tRNA synthetase, a crucial enzyme for protein biosynthesis, once taken up by bacteria through a siderophore uptake machineries, of which events lead to the growth inhibition of treated pathogens.Structurally, albomycin δ2 contains a few uncommon functionalities such as the thiofuranose ring and N4-carbamoyl group at the cytosine base. Intrigued by such unique structural features, we decided to pursue total synthesis of albomycin δ2. In addition, we are also planning to investigate the origin of its excellent antimicrobial activity as well as biosynthesis mechanisms of the thionucleoside formation.



Albomycin δ_2 R = $NCONH_2$
Albomycin ε R = NH
Albomycin δ_1 R = O

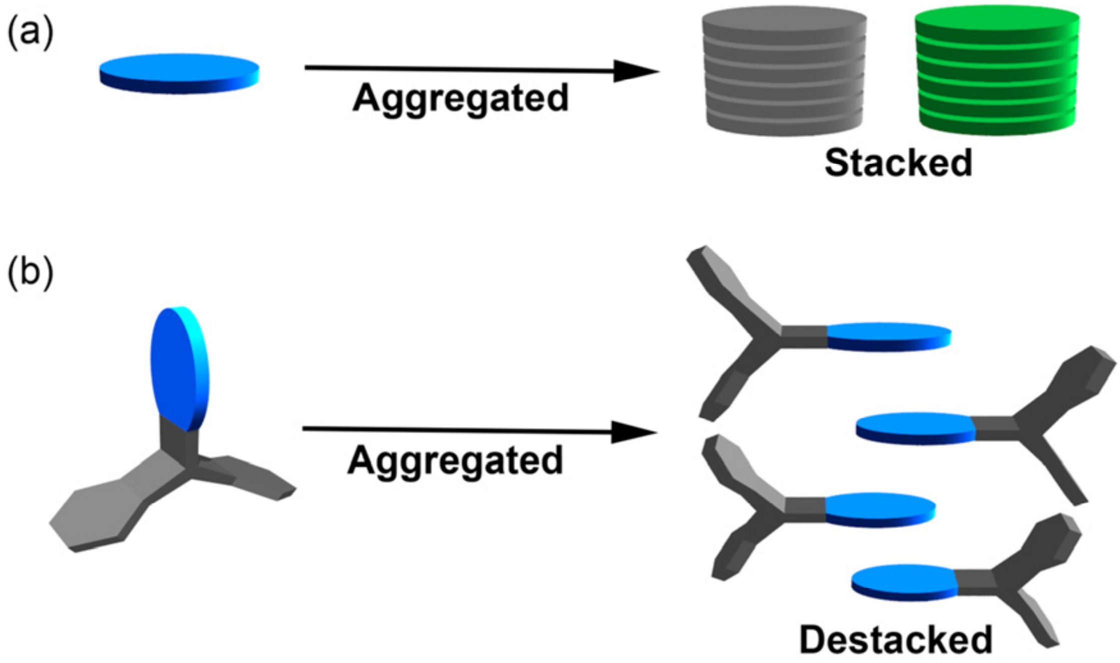
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-237**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Iptycene-Fused Triazoles: Three-Dimensional Aromatic Scaffold as a Destacker as well as a Regiocontroller

강태원 김홍식 이동환*

서울대학교 화학부

Solid-state organic fluorophores have wide applicability and solution processability. For most of the solid-state organic fluorophores, however, their photophysics deviates significantly from solution state properties. This is primarily due to strong intermolecular interactions in the condensed phase. It is challenging to design new solid-state organic fluorophores with desired emission properties since such intermolecular interactions are difficult to predict and control precisely. In order to overcome this problem, we have designed new organic solid-state fluorophores, triazoliptycenes, by integrating various N-2-aryltriazole fluorophores into the three-dimensional iptycene motif. Here, the iptycene scaffold effectively suppressed intermolecular π–π stacking interactions without compromising the inherent emission properties of the N-2-aryltriazole cores, as confirmed by both experimental and computational studies. Furthermore, the iptycene motif remarkably improved the regioselectivity of C–N coupling reaction by imposing significant stereoelectronic bias on the triazole ring. In sum, the three-dimensional aromatic scaffold of iptycene effectively functions as a regiocontroller in the synthesis as well as a destacker in the solid-state assembly. Both properties were exploited to produce a new class of solid-state light-emitters with tunable spectral window and high fluorescence quantum yields.


(a)
Aggregated
Stacked
(b)
Aggregated
Destacked

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-238**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile Synthesis and Nitric Oxide Inhibitory Activity of Aurones, Rugaurone A, Gramflavonoid A and Their Derivatives

KONGARADAMODAR 전종갑[1,*]

한림대학교 천연의학연구소 [1]한림대학교 화학과

Facile synthesis of natural aurones, rugaurone A (1a), gramflavonoid A (1b) and their novel derivatives (1c-1o) is accomplished in good to high yields with exceptional *Z*-selectivity (≥ 97%) from the commercially available starting materials. Herein, practically improved method was developed for the synthesis of common key intermediate, 5,6-dimethoxybenzofuran-3(2H)-one (5). Later, their nitric oxide (NO) production inhibition effects were estimated in lipopolysaccharide (LPS)-induced RAW-264.7 macrophages as an indicator of anti-inflammatory activity. All compounds exhibited weak to good strength against NO production with concentration-dependent manner and none of the compound showed significant cytotoxicity against macrophages at the highest (10 µM) concentration. The IC_{50} values are showed in the range from 3.39 to 19.55 µM. Among the 15 aurones synthesized in this study, 3 compounds that is compound 1g (63.98%) followed by compound 1o (49.07%) and rugaurone A (1a) (41.72%) showed the maximum inhibitory activity with respective IC_{50} values of 4.50 µM, 4.98 µM and 3.39 µM compared to L-NMMA (IC_{50} = 5.19 µM), which was used as a standard NO inhibitor. This study suggests that compounds 1g, 1o and 1a may serve as favorable structures for further development of NO production-targeted anti-inflammatory agents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-239**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient synthesis of 1,3-diarylpropanes and their *anti*-inflammatory effects

장하영 전종갑*

한림대학교 화학과

1,3-Diarylpropanes are important secondary metabolites of plants and exhibit diverse biological activities *viz.* antifungal, *anti*-inflammatory, anticancer, antiadipogenic, antitubercular and antimalarial to name a few. An efficient synthesis of diarylpropanes 1-5 is achieved from the commercially available starting materials and Claisen-Schmidt condensation and hydrogenation as key steps. Subsequently, we measured the anti-inflammatory effects of 1-5 by measuring the amount of nitric oxide (NO) which is one of the essential mediators of inflammation induced by lipopolysaccharide (LPS) in macrophage- derived RAW 264.7 cells. All the tested compounds significantly decreased NO production in a concentration-dependent manner except compounds 1, 3 and did not show notable cytotoxicity. The percentage of NO production inhibition ranged from 100.0% to 21.8% and from 40.8% to 27.2% at the highest (10 μM) and lowest (1 μM) concentrations, respectively. Of the 5 compounds (1-5) prepared in the present study, Compound 4 (hindsiipropane B) (100%; IC_{50} = 1.84 μM) possessed the most potent NO inhibitory activity which was even stronger than the positive control, L-NMMA (90.1%; IC_{50} = 2.73 μM) at 10 μM concentration and this finding was also further correlated by suppressed expression of LPS stimulated inducible NO synthase. Finally, Our study suggested that compound 4, holding a 1,3-diarylpropane scaffold with 3'',4''-dimethoxyphenyl and 3',4'-dihydroxy-2'-methoxyphenyl motifs could be considered as potential compound or lead compound for further development of NO production-targeted anti-inflammatory agents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-240**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and pharmacological evaluation of dihydrostilbenes as potent *anti*-inflammatory agents

박형진 전종갑*

한림대학교 화학과

As the synthesis of bioactive natural products and their analogues as potential NO inhibitors, we report an efficient synthesis and in vitro *anti*-inflammatory activity evaluation of dihydrostilbenes (1-5). In this, 1 (moscatilin) and 5 (aphyllal C) are natural dihydrostilbenes, isolated from *Dendrobium moscatum* and *Dendrobium aphyllum*, respectively. An efficient synthesis of dihydrostilbenes (1-5) is achieved from the commercially available starting materials and Wittig-Horner reaction, hydrogenation as key steps. Later, their nitric oxide (NO) production inhibition effects were evaluated in lipopolysaccharide (LPS)-induced RAW-264.7 macrophages as an indicator of *anti*-inflammatory activity. All the tested compounds significantly decreased NO production in a concentration-dependent manner except compound 2 and did not show notable cytotoxicity except compound 1. Compound 4 (75.5%; IC_{50} = 2.98 μM) at 10 μM concentration possessed the very good potent NO inhibitory activity and this finding was also further correlated by suppressed expression of LPS stimulated inducible NO synthase. Our study revealed that compound 4, a 1,2-dihydrostilbene scaffold with 3'',4''-dimethoxyphenyl and 3',4'-dihydroxy-2'-methoxyphenyl motifs could be considered as potential compound or lead compound for further development of NO production-targeted *anti*-inflammatory agents.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-241**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Natural C-methyl isoflavone and its derivatives

정종운 전종갑[1,*]

한림대학교 화학과, 응용화학연구소 [1]한림대학교 화학과

Isosideroxylin, a new C-methyl isoflavone, was isolated from the EtOAc extract of the leaves of *Leiophyllum buxifolium* and displayed antiproliferative effect against ER−MDAMB-231 cell lines and anticancer activity against ER+ MCF-7 breast cancer cell line and the NIH3T3 mouse fibroblast cell line. It also showed a selective antiproliferative effect against MDAMB-231 cells. We attempted the synthesis of isosideroxylin and its derivatives through enamino ketone formation followed by iodine promoted ring closure reaction and Suzuki coupling synthetic sequence. In addition, their *anti*-inflammatory effects were also investigated in lipopolysaccharide (LPS)-induced RAW-264.7 macrophages. All compounds exhibited significant inhibition of inflammatory mediated nitric oxide (NO) production with no cytotoxicity at 10µM concentration and IC_{50} values are found in the range from 10.17 to 33.88 µM.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-242**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient bipolar host materials based on phenyl silane and carbazole derivatives for blue phosphorescent OLEDs

주미라 양두리[1] **RAMANASKANDA BRAVEENTH POTHUPITIYA GAMAGESUDESH JAYASHANTHA** 채규윤[*]

원광대학교 화학과 [1]원광대학교 바이오나노화학과

A series of novel bipolar host materials based on silane and carbazole derivatives were successfully designed and synthesis. All materials were showed good thermal stabilities. Among these host materials diphenyldi(4-(3, 5-bis-carbazol-9-yl)phenyl silane (DM4CzDBPSi) exhibited higher glass transition temperature (197 ℃) and higher decomposition temperature at 5% weight reduction (535 ℃). Here we introduced silane group to mitigate the conjugation length which provided the higher triplet energy of 2.82 eV for DM4CzDBPSi. A blue phosphorescent organic light emitting diode based on FIrpic dopant was employed with DM4CzDBPSi as host material showed best device performance with maximum external quantum efficiency of 20.9% and a power efficiency of 41.28 Lm/W.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-243**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A synthetic approach to ^{18}F-labeled 2',3'-dideoxy-3'-fluoronucleoside containing an unnatural base

정수진 황길태*

경북대학교 화학과

Cancer cell proliferation is considered to be a useful prognostic indicator of tumor progression and remedial value. Until now, the molecular imaging with positron emission tomography (PET) is the most widely used to diagnose the cancer cell proliferation. It is a highly sensitive treatment plan and non-invasive technology that is ideally suited for pre-clinical and clinical imaging of cancer as quantifying and visualizing biochemical pathways in vivo.

Especially, radiolabelled nucleosides as PET probes are developed for early stage diagnosis and better management of oncology patients. The ^{18}F-labeled material is attractive because of its high resolution, chemical safety, sensitive detection and the easy measurement of drug concentration in vivo.

In this study we report the synthesis of 2',3'-dideoxy-3'-fluoronucleosides containing the unnatural base as a nucleobase, for example, pyridone, benzene, or isoquinolinone. One noteworthy feature here is that the introduction step of ^{18}F isotope to the 3' position of the nucleoside is applied in the final step. This synthetic strategy is expected to reduce the loss of radioactivity of ^{18}F -labeled 2',3'-dideoxy-3'-fluoronucleosides.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-244**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and fluorescent characteristics of oligodeoxynucleotides containing the 2'-deoxyuridine labeled with fluorene derivative under different pH conditions

<u>손예슬</u> 황길태*

경북대학교 화학과

The proton is one of the most important targets in cell metabolism process because intracellular pH plays critical roles in many cellular processes. Thus, monitoring of intracellular pH changes is very important to study function of cells and understand physiological and pathological process. Recently, many fluorescence probes and a variety of pH-sensitive nucleosides have been developed as a tool for monitoring of intracellular pH, however, DNA strands containing a pH-sensitive nucleoside have not been reported.

pH-sensitive DNA strands can be used as single nucleotide polymorphism (SNP) probe. The SNP is a variation at a single position in a DNA sequence among individuals and associated with certain diseases. These associations allow scientists to look for SNPs in order to evaluate an individual's genetic predisposition to develop a disease. If DNA strands are developed as a sensor for detecting pH changes, they can available in the public databases makes studies of association and fine mapping of disease loci very practical.

In this study, we synthesized oligodeoxynucleotides bearing the 2’-deoxyuridine labeled with a fluorene derivative as a pH-sensitive SNP probe and examined their photophysical properties under different pH conditions. We are expecting that these DNA strands can be a useful tool for studying a variety of diseases by monitoring pH changes in a living system.

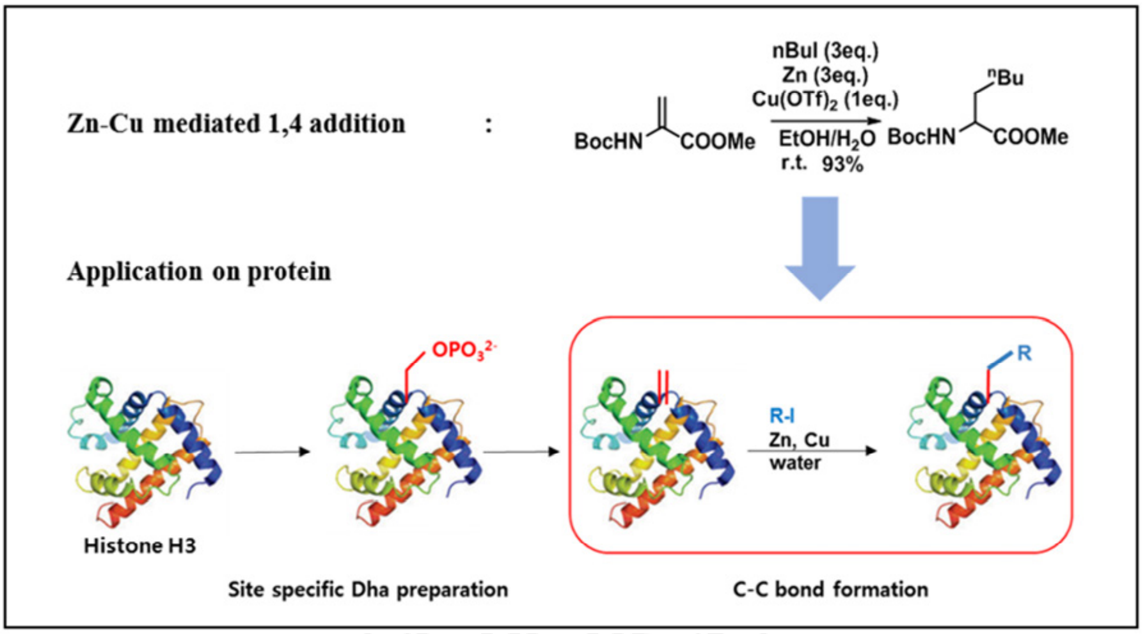
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-245**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of zinc-copper mediated C-C bond forming reaction of Dehydroalanine in water and application to the site specific protein post-translational modification(PTM)

<u>김리라</u> 이희윤*

KAIST 화학과

Chemical post-translational modification of proteins would facilitate the understanding of many essential biological processes including cell signalling. However, their functional studies has been limited since only limited number of chemical tools have been developed to produce diverse protein diversity. We optimized the metal mediated carbon-carbon bond formation between alkyl iodide and α,β-unsaturated carbonyl compound(Dha) [1] to realize the coupling of dehydroalanine (Dha) [2] and alkyl iodide with zinc and copper under aqueous environment. This reaction was successfully applied to the authentic PTM histone H3 modification to afford the site specific modified H3K79 formylation, acetylation, and methylations.The new method would offer a powerful tool for diverse authentic PTMs of protein and researches in chemical biology or bioengineering fields.Reference 1.(a) J. L. Luche, C. Allavena, C. Petrier, C. Dupuy, Tetrahedron Lett, 1988, 29, 5373-5374. (b) T. Huang, C. C. K. Keh, C. J. Li, Chem. Comm., 2002, 2440-2441 (c) B. H. Lipshutz, S. Huang, W. W. Y. Leong, G. Zhong, N. A. Isley, J. Am. Chem. Soc. 2012, 134, 19985– 199882.(a) H. S. Park, M. J. Hohn, T. Umehara, L. T. Guo, E. M. Osborne, J. Benner, C. J. Noren, J. Rinehart, D. Söll, Science, 2011, 333, 1151-1154 (b) S. Lee, S. Oh, A. Yang, J. Kim, D. Söll. D. Lee, H. S. Park, Angew.Chem.Int.Ed., 2013, 52, 5771. (c) Y. Oda, T. Nagasu, B. T. Chait, Nat. Biotech., 2001, 19, 379


Zn-Cu mediated 1,4 addition :
BocHN
COOMe
nBuI (3eq.)
Zn (3eq.)
Cu(OTf)$_2$ (1eq.)
EtOH/H$_2$O
r.t. 93%
^{n}Bu
BocHN
COOMe
Application on protein
Histone H3
OPO$_3^{2-}$
R-I
Zn, Cu
water
R
Site specific Dha preparation
C-C bond formation

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-246**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of bio-based polyols for the preparation of high-end polyurethane

김미진 박철오[1] 윤선혜[2] 김성덕[3] 부충헌[3] 정동운[3] 김민규[2,*]

(주)세호 연구개발 [1]주)세호 연구개발부 [2](주)세호 연구개발부 [3]원광대학교 화학과

Bio-based succinic acid has attracted as one of the new bio-based chemicals for the preparation of polyurethane. Renewable bio-based polyols with good product properties such as hydroxyl number, acid value, viscosity, moisture, functionality, color, etc. can be synthesised from the bio-based succinic acid for the preparation of high-end polyurethane.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-247**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Hydrophobic Tag-assisted liquid phase systhesis of peptide nucleic acids

박지혜 김초롱 김은택 홍인석*

공주대학교 화학과

PNA Oligomers have been made using the SPPS methods until now. However, this method consumed large amounts of PNA Monomer, and had scale up limitations. In order to overcome these problems, we introduced a hydrophobic Tag-assisted liquid phase peptide synthesis. Tag is a material that supports peptide-synthesis in liquid phase. Tag has the advantage of being able to easily remove the other by-products in the polar solvent such as MeCN, MeOH because it consists of long alkyl chains. Several short PNA oligomers were successfully synthesized by this methods, and identified.

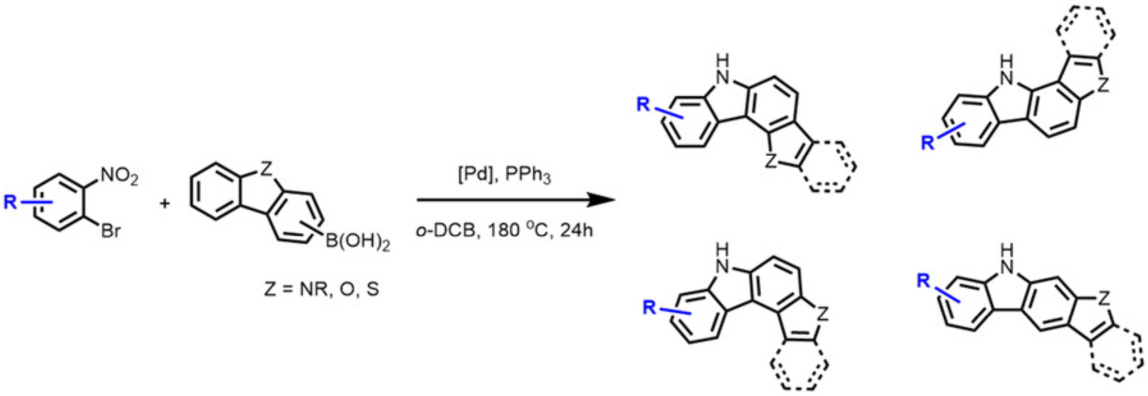
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-248**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthetic Study of Heteroaryl-annulated Carbazoles via tandem Suzuki cross-coupling and reductive Cadogan cyclization

김형석 우상국*

울산대학교 화학과

We have developed a highly efficient synthetic methods of heteroaryl-annulated carbazoles that are sequential C-C/C-N bond formation via Suzuki cross-coupling and Cadogan cyclization using commercially available or easily preparable starting materials. The developed method is compatible with electron neutral, rich and deficient substrates.



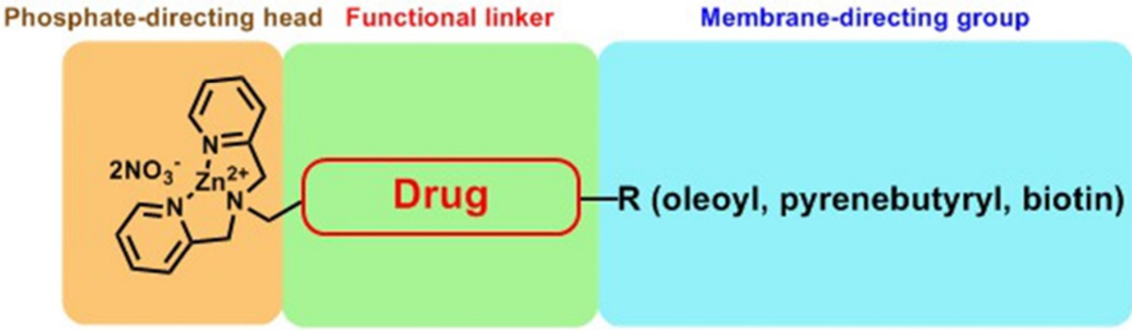
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-249**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Novel siRNA Transporters with The Zinc(II)dipicolylamine Head and A Functional Linker

한정화 금교창[1] 방은경[2,*]

상명대학교 화학과 [1]한국과학기술연구원(KIST) 케모인포메틱스연구센터 [2]한국과학기술연구원(KIST) 뇌의약연구단

RNA interference is currently the most efficient method for gene down-regulation. However, the poor membrane permeability of small interfering RNAs (siRNAs) remains a hurdle for their clinical applications as RNAi agents. Among the reported delivery systems for siRNAs, cationic amphiphiles were the earliest and the most popular delivery system for increasing the cellular uptake of siRNAs. Conventional cationic amphiphiles typically comprise a cationic head, a linker, and a hydrophobic tail. In the previous study, we developed coordinative amphiphiles for use as novel siRNA transporters.1 We replaced the cationic head with zinc(II)-dipicolylamine complex (Zn/DPA) as a phosphate-directing group, and used various membrane-directing groups in the place of the hydrophobic tails. The Zn/DPA head itself exhibited moderate transfection efficiency, and its combination with a membrane-directing group—oleoyl, pyrenebutyryl, or biotin—enhanced the delivery efficiency without imparting significant cytotoxicity. Here we replaced the simple linker with a functional linker—such as a commercial drug. This functional coordinative amphiphiles could deliver siRNAs into cells and function as a drug in the cell at the same time. We designed and synthesized several candidates, and studied their property as both a siRNA transporters and a drug.References1. Kim, J. B.; Lee, Y. M.; Ryu, J. Y.; Lee, E. J.; Kim, W. J.; Keum, G. C.; Bang E. K. Bioconjugate Chemistry 2016, DOI: 10.1021/acs.bioconjchem.6b00260.


Phosphate-directing head
Functional linker
Membrane-directing group
2NO3-
Zn2+
N
Drug
R (oleoyl, pyrenebutyryl, biotin)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-250**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A new series of antioxidant system of resveratrol analogue

임현민 이정태*

한림대학교 화학과

[1]Resveratrol, a natural stilbene derivate that exists in numerous foods, has attracted considerable attention over the past decades owing to its multiple beneficial properties, such as chemopreventive and antitumor activities.A series of the benzofuran derivatives were synthesized and characterized. These compounds will be tested as antioxidants and anti-inflamatory agents. Reference[1]Simone, F. *Drug Discovery Today*. 2010. 15. 17-8

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-251**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Antioxidant Activity of Resveratrol Derivatives

남기윤 이정태*

한림대학교 화학과

Resveratrol (3,5,4'-*trans*-trihydroxystilbene) is a well-known natural product that has antioxidant activity. Therefore, various resveratrol derivatives have been synthesized to enhance antioxidant activity. Here, we report the synthesis of expanded resveratrol analogues using Wittig-Horner reaction. The antioxidant activity of these newly synthesized compounds has been measured by ABTS assay, and IC_{50} values of these compounds were obtained.

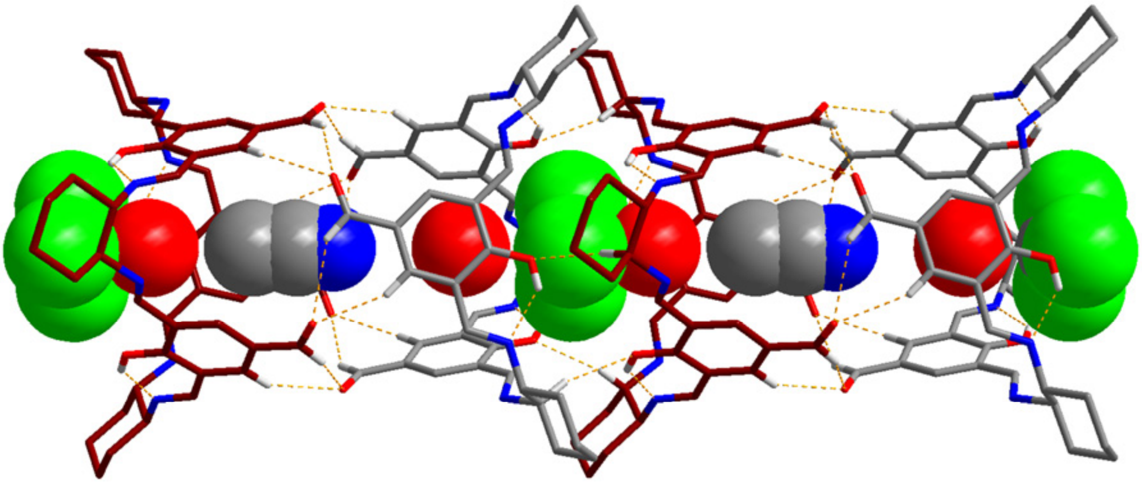
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-252**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Tube-type Supramolecular Architecture Constructed by H-bonds between Calixsalens

황지은 이은지[1] 허정석* 박기민[2,*]

충남대학교 화학과 [1]경상대학교 화학과 [2]경상대학교 기초과학연구소

The design and synthesis of macrocyclic Schiff-base ligands are fascinating areas of research owing to their use as models for biological metal-binding sites and their ability to form metal complexes with catalytic properties. Furthermore, macrocyclic Schiff-base ligands with phenolic groups have been of great importance in macrocyclic chemistry because they can selectively chelate certain metal ions depending on the number, type and position of their donor atoms, the ionic radius of the metal centers, and the coordinating properties of the counterions. In order to develop macrocyclic Schiff-base ligands with phenolic groups, we synthesized firstly 2,4,6-triformylphenol in high yield. The [3 + 3] cyclocondensation of 2,4,6-triformylphenol with racemic *trans*-1,2-diaminocyclohexane results in formation of triangular vase-like hexaimines, called calixsalens, as macrocyclic Schiff-bases with phenolic groups (See the figure below). In the solid state, interestingly, the obtained calixsalens are linked to each other by several H-bonds, leading to the formation of a tube-type supramolecular architecture. Herein, we present its crystal structure and physical properties.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-253**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Phase-Transfer-Catalyzed Enantioselective Aza-Michael Reactions: Synthesis of Chiral Pyrazoles

최다민 조창우*

경북대학교 화학과

Pyrazole is important skeleton that exhibit a variety of interesting biological activities and thus have found application in the development of pharmaceuticals such as Celebrex and Zoniporide. However, the use of pyrazole as the *N*-centered heteroaromatic nucleophile remains almost unexplored in organocatalytic asymmetric reactions, in spite of the importance of pyrazole as optically pure *N*-heteroaromatic pharmacophores in biologically active natural products. Here, the use of pyrazoles as the *N*-centered heteroaromatic nucleophiles in the organocatalytic asymmetric aza-Michael reactions of enones will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-254**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Diastereoselective Synthesis of Chiral 2-Alkylated 3,3-Dinitroazetidine Derivatives

하헌종 김승희[1] 김진석[2] 조창우[*]

경북대학교 화학과 [1]국방과학연구소 4본부2부 [2]국방과학연구소 4본부 2부

3,3-Dinitroazetidine derivatives constitute an important class of energetic materials, with inherently high energies resulting from their strained ring systems and nitrogen contents. In particular, 1,3,3-trinitroazetidine, with its higher nitrogen content, has received considerable attention as a potential high performance melt-castable explosive in the defense and explosives industries. Recently, as an example of possible medical applications of energetic materials, 1-bromoacetyl-3,3-dinitroazetidine was developed as a novel class of anticancer agent and is currently in a phase I clinical trial. Because of this versatility of 3,3-dinitroazetidine in the fields of both drug discovery and energetic materials, we planned to synthesize a variety of 2-alkylated 3,3- dinitroazetidine derivatives, especially chiral 2-alkyl-3,3-dinitro-1-tosylazetidines. To the best of our knowledge, the synthesis of chiral 2-substituted 3,3-dinitroazetidine derivatives has never been reported despite their versatile applicability in both materials and medicinal chemistry areas. Therefore, we report the asymmetric synthesis of chiral 2-alkylated 3,3-dinitroazetines via a diastereoselective aza-Henry reaction followed by Mitsunobu cyclization.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-255**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enantioselective Synthesis of Chiral *N*-Substituted 3,3-Dinitroazetidine Derivatives by Phase-Transfer-Catalyzed Aza-Michael Reaction

서지환 조창우*

경북대학교 화학과

Azetidines are an important class of saturated aza-heterocycles found in naturally occurring organic molecules and pharmaceuticals showing a variety of potent biological activities. For this reason, azetidine synthesis has received considerable attention. In particular, the synthesis of optically pure azetidines has been a subject of active research. However, while catalytic enantioselective synthesis of chiral *C*-substituted azetidines has been widely researched, the corresponding synthesis of chiral *N*-substituted azetidines, which bear a stereogenic carbon center at the α-position of the nitrogen atom, remains unexplored. Despite the significance of the chiral *N*-substituted azetidines as optically pure *N*-heterocyclic pharmacophores in bioactive compounds, the use of azetidines as *N*-centered nucleophiles in catalytic enantioselective aza-Michael reactions has not been reported. Herein, we report the efficient and highly enantioselective phase-transfer-catalyzed aza-Michael reaction of 3,3-dinitroazetidine, as a *N*-centered nucleophile, to α,β-unsaturated ketones; to the best of our knowledge, this would be a first example of the use of azetidines as *N*-centered nucleophiles in catalytic enantioselective aza-Michael reactions. The enantioselective phase-transfer-catalyzed aza-Michael reaction affords chiral *N*-substituted 3,3-dinitroazetidines in good yields and excellent enantioselectivities.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-256**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

G-C와 C-G Morpholino Glycine Nucleotide 이합체의 합성

김도영 전근호[1,*]

숭실대학교 화학과 [1]숭실대학교 화학

올리고뉴클레오티드를 기반으로 한 유전자 발현의 억제 기술, 즉 안티센스 기술은 신약개발에 있어서 중요 기술로 주목받고 있다. 최근 PNA(Peptide Nucleic Acid) dimer 가 염기들간의 상호작용과 Wastson-Crick 형태의 수소결합으로 인한 자가 정렬에 의해 특정구조를 형성하여 voltage dependent electroluminescence 와 excitation dependent fluorescence 의 특성을 지니는 것이 알려졌다. 본 연구에서는 Morpholine nucleotide dimer 를 합성하여 PNA 와 유사한 광학특징을 나타나는지 알아보기 위하여 Cytosine 과 Guanine 을 염기로 갖는 Morpholine dinucleotide 를 합성했다. 더 나아가 기존의 PMO(Phosphoroamidate morpholino oligonucleotide)에서 chiral center 로 인한 이성질체가 만들어지는 현상을 극복하기 위하여 Glycineamide linkages 를 이용하여 Morpholino glycine dinucleotide (G-C, C-G)를 합성했다.

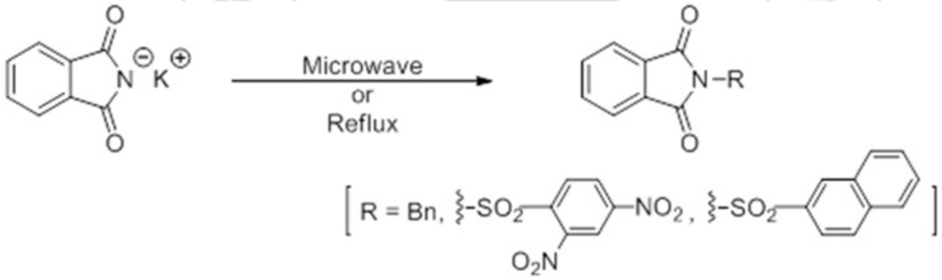
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-257**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

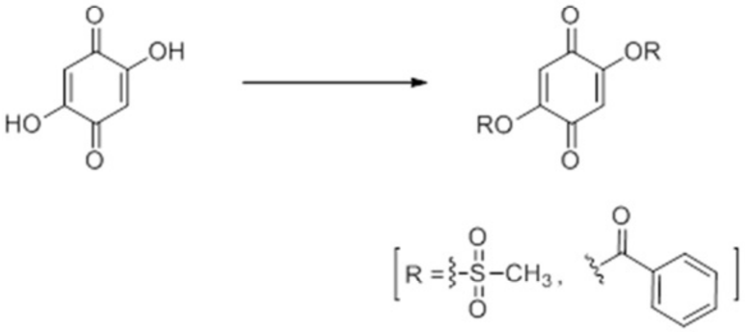
Preparation and Electrochemical Investigation of Phthalimide and Quinone Derivatives: Apply to Redox Flow Battery

김미형 안철진*

창원대학교 화학과

Recently phthalimide and quinone derivatives are interesting to organic anolyte in redox flow batteries(RFBs) for offering the possibility of wide potential windows. Herein we report the investigation on relationship between electrochemical properties of phthalimide and quinone derivatives. To do this we prepared phthalimide and quinone derivatives and investigated CV results depending on their different functional group.





일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-258**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

화학적으로 변형된 사이토신 염기의 합성과 변형된 사이토신과 구아닌염기를 이용한 펩타이드 핵산 GC 이합체의 합성

이영덕 전근호[1,*]

승실대학교 화학과 [1]승실대학교 화학

안티센스 기술을 응용한 치료제의 개발은 다양한 분야에서 연구가 계속 진행되고 있고, 유망한 안티센스 약물 후보 물질을 찾기 위하여 다양한 올리고 뉴클레오티드들이 개발되고 있다. 생체 안정성과 세포투과성, 독성등과 같은 기존 안티센스 물질들의 한계들을 극복하기 위하여 펩타이드 핵산은 지난 20 년간 지속적으로 연구되어 왔다. PNA(Peptide or Polyamide Nucleic Acid) 유도체는 achiral 하고 전하를 띄지 않는 backbobne 을 가지고 있고, sense DNA, RNA 에 대한 강한 결합력과 특수성을 가지고 있다. 최근 연구들에 따르면 구아닌을 포함한 di-PNA (GC, CG, GG)는 self assembly 를 이룬다고 보고 된 바 있으며, 우리는 이 근거를 바탕으로 화학적으로 변형된 사이토신을 합성하고, 변형된 사이토신을 이용한 GC di-PNA 이합체를 합성했다. 화학적으로 변형된 사이토신은 G-clamp 가 가능하며, 이를 통해 기존에 보고 되었던 화학적으로 변형 되지 않은 사이토신을 이용한 GC di-PNA 보다 더욱 self assembly 를 잘 이룰 것으로 예상하며 특이한 전기적 특성을 나타낼 것으로 기대한다.

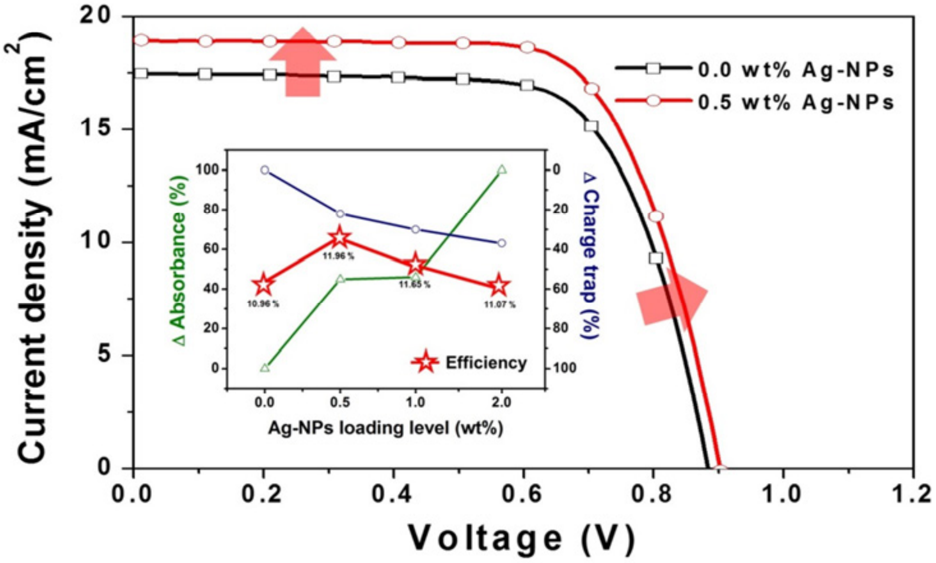
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-259**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Correlations of Optical Absorption, Charge Trapping, and Surface Roughness of TiO_2 Photoanode Layer Loaded with Neat Ag-NPs for Efficient Perovskite Solar Cells

양동욱 김성현* 홍종인*

서울대학교 화학부

We systematically investigated the effect of Ag-NPs on the power conversion efficiency (PCE) of perovskite solar cells (PSCs). Neat, spherical Ag-NPs were embedded into the TiO_2 photoanode layer. The plasmonic effect of the Ag-NPs strongly enhanced the incident light absorption over a wide range of the visible wavelength region in addition to the inherent absorbance of the perovskite sensitizer. The low conduction energy level of the Ag-NPs compared to that of TiO_2 provides trap sites for free charge carriers. Thus, the correlation between the enhancement of the optical absorption and the number of charge traps provided by the Ag-NPs is critical to determine the device performance, especially current density (J_{sc}) and PCE. This is confirmed by the quantitative comparison of the incident light absorption and the time-resolved photoluminescence decay according to the loading levels of the Ag-NPs. The absorption enhancement from 380 to 750 nm in the UV−visible spectrum is proportional to the increase in the loading levels of the Ag-NPs. However, the J_{sc} increases with the device with 0.5 wt % Ag-NPs and gradually decreases with increases in the loading level above 0.5 wt % because of the different contributions to the absorbance and the charge trapping by different Ag-NP loading levels. In addition, the suppression of the surface roughness with dense packing by the Ag-NPs helps to improve the Jsc and the following PCE.Consequently, the PCE of the PSC with 0.5 wt % Ag-NPs is increased to 11.96%. These results are attributed to the balance between increased absorbance by the localized surface plasmon resonance and the decreased charge trapping as well as the decreased surface roughness of the TiO_2 layer with the Ag-NPs.


Current density (mA/cm^2)
20
15
10
5
0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Voltage (V)
0.0 wt% Ag-NPs
0.5 wt% Ag-NPs
Δ Absorbance (%)
100
80
60
40
20
0
Δ Charge trap (%)
0
20
40
60
80
100
10.96 %
11.96 %
11.65 %
11.07 %
Efficiency
0.0
0.5
1.0
2.0
Ag-NPs loading level (wt%)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-260**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Photoluminescent and Electrochemiluminescent Dual Signaling Probe for Fluoride Detection based on a Ruthenium (II) Complex

YU SUH YOUNG 홍종인*

서울대학교 화학부

Anion detection is considered as attractive topic because of their important role in chemistry and biology. The fluoride (F_{-}), related with dental caries prevention or osteoporosis treatment, is a vital element in living bodies. However, a high intake of fluoride causes side effects such as fluorosis or urolithiasis. Therefore, it is needed to develop effective methods that can monitor fluoride ion level.Herein, we developed a heteroleptic ruthenium (II) complex as a chemodosimetric fluoride sensor using changes on photoluminescent (PL) and electrogenerated chemiluminescent (ECL). The ruthenium II) complex exhibits phosphorescent decrease of emission intensity and red shift of emission wavelength only toward fluoride ion. Moreover, the probe shows similar ECL changes – decrease of ECL intensity and shift of oxidation potential – taking advantage of the electrochemical properties of the ruthenium (II) complexes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-261**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Transition-Metal-Free Regioselective Alkylation of Pyridine N-Oxides Using 1,1-Diborylalkanes as Alkylating Reagents

조우현 김정훈 최서영 조승환*

POSTECH 화학과

We developed an unprecedented base-promoted deborylative alkylation of pyridine N-oxides using 1,1-diborylalkanes as alkyl sources. The reaction proceeds efficiently for a wide range of pyridine N-oxides and 1,1-diborylalkanes with excellent regioselectivity. The utility of the developed method is demonstrated by the sequential C-H arylation and methylation of pyridine N-oxides. The reaction also can be applied for the direct introduction of a methyl group to 9-O-methylquinine N-oxide, thus it can serve as a powerful method for late-stage functionalization.

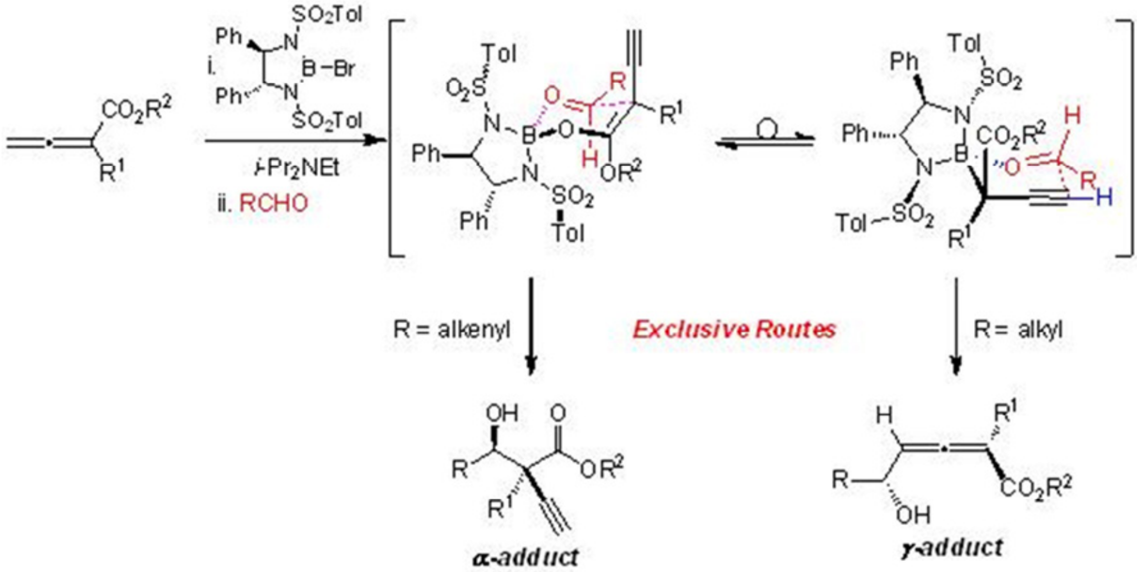
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-262**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Governing Factors for the Regulation of Alpha vs Gamma Asymmetric Addition Routes of Allenoates with Aldehydes

오창화 이지은[1] 권영은[1] 김지민[*] 유찬모[1,*]

전남대학교 화학과 [1]성균관대학교 화학과

Among a variety of synthetic methods for the construction of cyclic compounds, reactions involving the use of Lewis acid catalysts are some of the most attractive methodologies. In this regard aldol reaction of carbonyl functionalities using chiral auxiliaries or catalysts led to significant developments in the area of asymmetric synthesis. As part of our investigations utilizing allenoates as versatile substrates for asymmetric carbonyl additions, we present herein our discovery of control elements to regulate selective formation of alpha adduct or gamma adducts from the reaction of allenoates with aldehydes as shown in following scheme, which allows in good yields with high levels of stereoselectivity as shown following Scheme. We will present regulation factor for reactions, and also the scope of reaction and stereoselectivity.


i.
Ph
Ph
SO2Tol
B–Br
SO2Tol
i-Pr2NEt
ii. RCHO
CO2R2
R1
Tol
O2S
O
R
R1
Ph
N
B
O
H
OR2
N
SO2
Ph
Tol
Ph
Tol
SO2
Ph
N
CO2R2
H
N–B
O
R
H
Tol–SO2
R1
R = alkenyl
Exclusive Routes
R = alkyl
OH
O
R
OR2
R1
α-adduct
H
R1
R
OH
CO2R2
γ-adduct

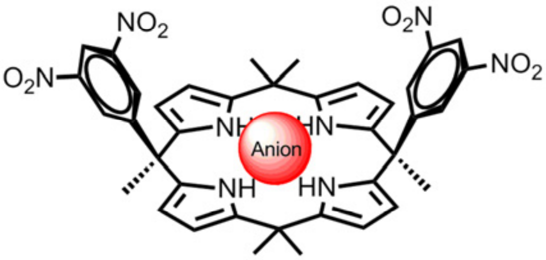
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-263**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Anion-π interaction in meso-dinitrophenyl functionalized calix[4]pyrrole isomers

김아정 박정수*

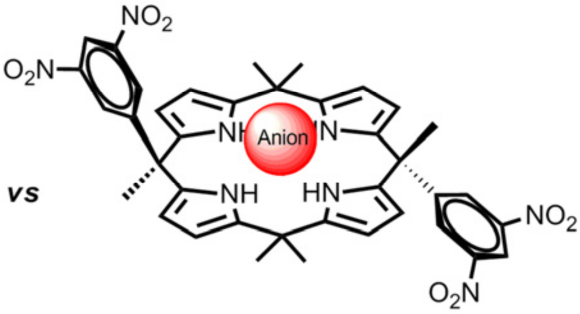
숙명여자대학교 화학과

For the construction of synthetic anion receptors, various non-covalent interactions have been employed. These include Coulombic attractions, Lewis acid-base pairing, metal coordination, dipole-anion, multiple hydrogen and halogen bonding, anion-π interaction and various combinations thereof.[1] Among these, anion-π interactions have been recently recognized and the focus of intense studies.[2] Herein, we investigate anion-π binding modes in a *cis*-isomer of 3,5-dinitrophenyl-substituted calix[4]pyrrole with various anions (F^-, Cl^-, Br^-, I^-, NO_3^-, AcO^-, HCO_3^-, HSO_4^-, and $H_2PO_4^-$) via X-ray crystallographic analyses and compare its binding affinities with those of the corresponding *trans*-isomer. The obtained results from these solid-state analyses clearly confirmed that all tested anions resides inside of cavity regardless its size and geometry. It is also believed that these structural analyses can provide useful insights into understanding the sandwich-type π-anion-π interactions. The receptor 1, capable of bidentate anion-π interaction, shows higher affinities across the board than does the receptor 2. Especially significant enhancement for $H_2PO_4^-$ was observed.References 1. (a) R. Martínez-Máñez and F. Sancenón, Chem. Rev., 2003, 103, 4419; (b) A. Andrievsky, F. Ahuis, J. L. Sessler, F. Vögtle, D. Gudat and M. Moini, J. Am. Chem. Soc., 1998, 120, 9712;2. (a) M. Mascal, A. Armstrong and M. D. Bartberger, J. Am. Chem. Soc., 2002, 124, 6274;



1, Sandwich anion-pi interactions

vs



2, Single anion-pi interaction

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-264**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Palladium Catalysts on activated Carbon Supports with different Structure and Surface Chemical Properties

박희정 염을균[1,*]

한국기초과학지원연구원 서울서부센터 [1]충남대학교 화학과

A number of activated carbons produced from beach, peat, coconut shell, and by pyrolysis of hydrocarbons have been subjected to treatment with oxygen, chlorine, hydrogen or ammonia at elevated temperatures to get a representative series of catalyst supports differing in porous structure and surface chemistry. Palladium was deposited from anionic (H_2PdCl_4), neutral ($Pd(OAc)_2$, in acetone), and cationic ($[Pd(NH_3)_4](NO_3)_2$) complexes. Temperature-programmed reduction, CO chemisorption, and testing in olefin hydrogenation were used to study the possible effects of preparation variables. The origin of the carbon support and the temperature of the catalyst reduction with hydrogen proved to have a profound influence on the properties of the catalysts.

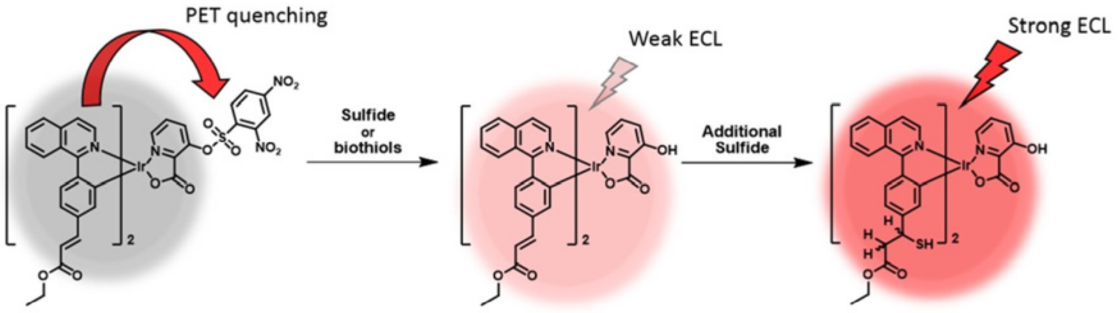
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-265**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Duel-quenching ECL probe with a High Turn-on Ratio for Sulfide Based on Cyclometalated Ir(III) Complex

김훈준 홍종인*

서울대학교 화학부

Electrogenerate chemiluminescence (ECL) refers to a light-emitting process by which chemical species undergo homogeneous electron transfer reactions at the surface of the working electrode in a solution. ECL-based chemosensors are powerful candidates for point-of-care-testing (POCT) due to their simple sensing processes and easy handling. Thus far, most ECL sensing systems have been developed, some of which are commercially available. However, ECL detection of small molecules is still a great challenge because most of ECL detection methods have been developed via specific biomacromolecular recognition such as antibody-antigen and aptamer-protein interactions. Herein, we introduce new ECL chemosensors for sulfide based on cyclometalated Ir(III) complexes. Probe 1 has two reaction sites, α,β-unsaturated ester (acrylate) moiety in the main ligand and 2,4-dinitrobenzenesulfonyl (DNBS) group in the ancillary ligand. The acrylate units reacted with sulfide selectively, inducing phosphorescence and ECL enhancement in the blue-shifted region. In addition, the DNBS group, a well-known PET quencher which can be cleaved by sulfide and other biothiols such as cysteine or homocysteine, was introduced for quenching the emission of probe itself. Probe 1 enabled sensitive and selective detection of sulfides by the introduction of two reaction sites in a single molecule. Details of synthesis, photophysical and electrochemical studies will be presented.


PET quenching
NO_2
NO_2
Sulfide
or
biothiols
Weak ECL
OH
Additional
Sulfide
Strong ECL
OH
SH
N
Ir
O
2

1   **1**-S^{2-}

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-266**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-Step Immobilization of Glucose Oxidase on Mesoporous Silica using Methallylsilane Coupling Reagent

정희태 전철호*

연세대학교 화학과

Immobilization of enzymes onto inorganic materials such as silica support has received considerable attention because of wide applications in biological science. Several methods for enzyme immobilization have been proposed including multistep grafting and adsorption immobilizations, etc. which have many drawbacks like poor immobilization of active site and facile leaching. In this report, the efficient one-step covalent bonding immobilization method of enzyme GOx (Glucose Oxidase) onto mesoporous silica is described. Immobilization of GOx onto silica surface is carried out by reacting GOx with NHS-ester-functionalized methallylsilane as a coupling reagent under various organic acid at 0 ^{o}C. The reaction is believed that lysine residue of GOx reacts with NHS-ester group of coupling reagent and organic acid promoted the reaction of the methallylsilane group of coupling reagent with silanol group of mesoporous silica surface. Loading efficiencies of GOx can be measured by spectroscopic method by determining H_2O_2, generated from the reaction of immobilized GOx with β-D-glucose.

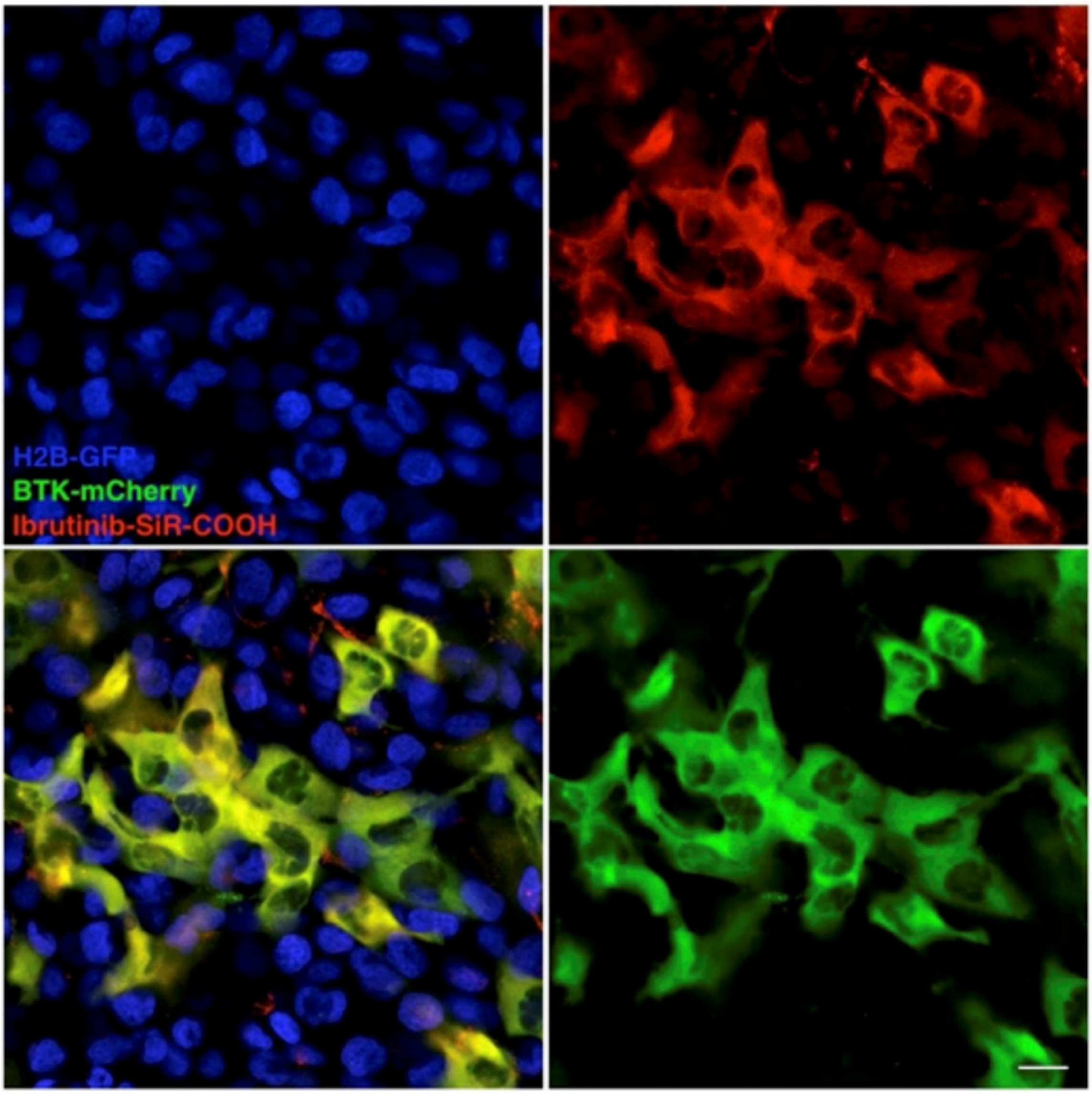
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-267**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of Companion Imaging Probe for In vivo study

김은하

아주대학교 분자과학기술학과

Drug development often fails at late stages after significant cost and time investment. Since target-to-hit and hit-to-lead process are based on biochemical/cell-based in vitro assay system, the processes does not guarantee in vivo efficacy of lead compounds. Moreover in the later stages of drug development quantitative mechanistic understanding at the molecular and cellular level is challenging to attain. As such, the inability to determine drug behavior and downstream effects in vivo limits our understanding of drug pharmacology and is a major impediment to developing 'first-in-class' medicines. To this end, new molecular biology tools which can fill this gap between in vitro and in vivo are needed to study how drugs work in vivo and when/how they fail. Fulfil this unmet need, we have been developed companion imaging probes (CIPs) for high-resolution intravital microscopy imaging techniques to study pharmacokinetic (PK)/pharmacodynamics (PD) in vivo. The CID can be obtained simply by conjugating fluorochrome to known clinical drugs. Contrary to the popular belief, however, the fluorochrome is not an inert color tag but is a molecule that can respond to environmental changes or interact with biomolecules. Furthermore chemical properties of fluorescent compound can significantly influence the fluorescent conjugates. Therefore molecular level understanding of the relationship between chemical structure and photophysical property will provide a rational molecular design principle for the development of novel CIDs. In this seminar, how understanding about structure-photophysical property relationship (SPPR) of fluorochrome can help to develop CID will be discussed with case study about Silicon-rhodamine fluorochrome and Bruton's Tyrosine Kinase inhibitor, Ibrutinib.


H2B-GFP
BTK-mCherry
Ibrutinib-SiR-COOH

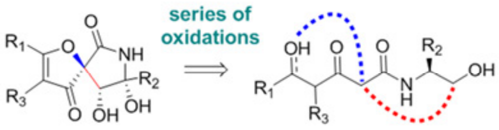
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-268**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

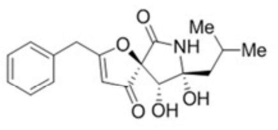
Biomimetic Total Synthesis of Berkeleyamide D

조덕희 한순규*

KAIST 화학과

Biomimetic total synthesis of berkeleyamide D is described. In 2004, Snider and co-workers reported a novel biomimetic route to 3-acyl-5-hydroxy-3-pyrrolin-2ones.1 Inspired by this biomimetic sequence, our group envisioned the synthesis of berkeleyamide D. We seek to construct the oxazaspirocyclic core of berkeleyamide D from a linear precursor via a series of oxidation processes. Our synthetic strategy will form the basis for the synthesis of various natural products which contains the oxa-azaspirononenedione core.





berkeleyamide D
inhibits matrix metalloproteinase-3
and caspase-1

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

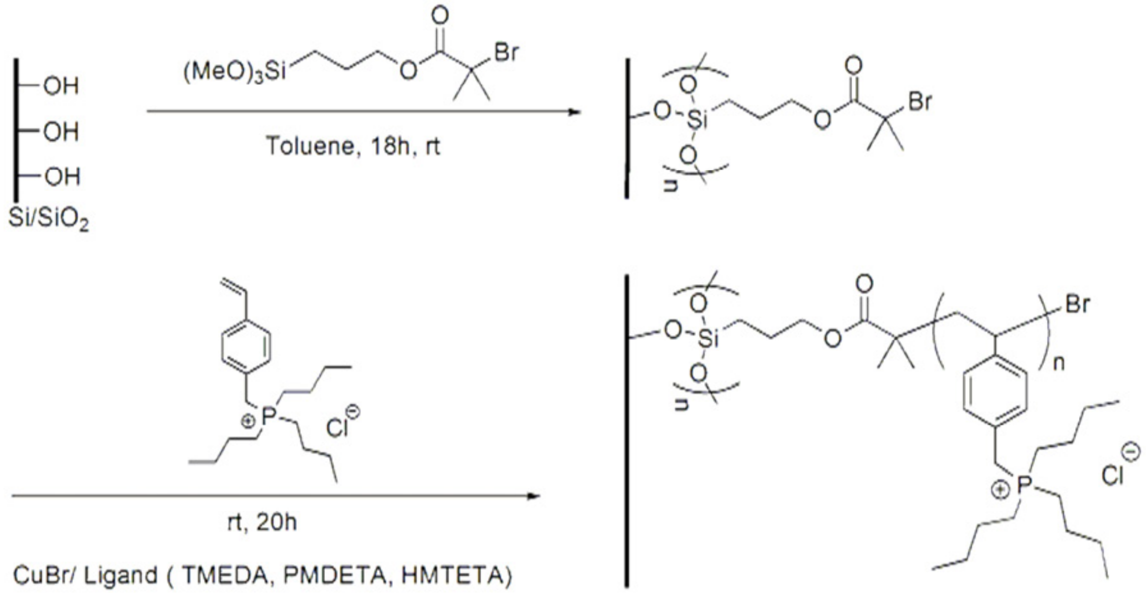
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-269**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ligand-mediated Surface Grafting of Bactericidal Phosphonium Salts via Atom Transfer Radical Polymerization

연도경 조우경*

충남대학교 화학과

The use of medical tools and equipment that are contaminated by bacteria can cause the mortality and infections of patients in hospital.1 One of methods to suppress bacterial contamination on surfaces is to kill bacteria by disrupting cell membrane once they adhere to surfaces. Herein we aim to graft the bactericidal polymer from a surface via atom transfer radical polymerization (ATRP) and pursue to optimize the polymer grafting by the control of aliphatic ligand. As a bactericidal material, we used phophonium salt that showed higher bactericidal activity2 than the polymeric quaternary ammonium salts, which have been widely used as bactericidal materials.3,4 Phosphnium salt monomer, tributyl-(4-vinylbenzyl)phosphonium chloride was synthesized by a single step. The polymeric phosphonium salt was grafted from silicon dioxide (SiO2) substrate by varying the reaction conditions. The polymer grafting was controlled by using three different aliphatic ligands such as N,N,N′,N′-Tetramethylethylenediamine (TMEDA), N,N,N′,N″,N″-Pentamethyldiethylenetriamine (PMDETA), and 1,1,4,7,10,10-Hexamethyltriethylenetetramine (HMTETA). The surface-grafted polymeric films were characterized by ellipsometry, contact angle goniometry, X-ray photoelectron spectroscopy, and atomic force microscopy. The polymer grafting was controllable depending on the used ligand, and the grafted polymeric film was the thickest when PDMETA was used.


OH
OH
OH
Si/SiO$_2$
(MeO)$_3$Si
O
Br
Toluene, 18h, rt
O
Si
n
rt, 20h
CuBr/ Ligand (TMEDA, PMDETA, HMTETA)
P
Cl
n
Br

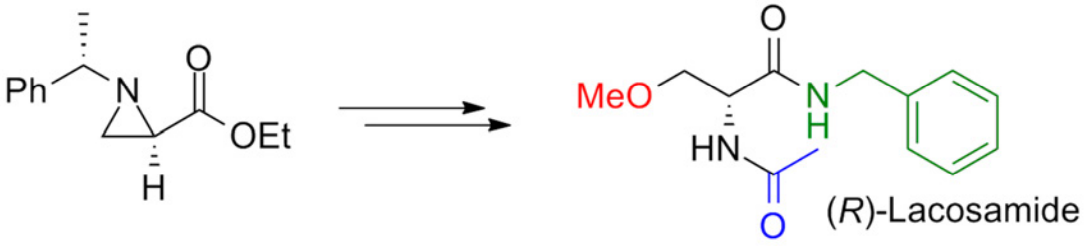
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-270**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Lacosamide (Vimpat) and Its Derivatives from Aziridine-(2*S*)-carboxylate

정현수

한국 외국어 대학교 화학과

An efficient and scalable synthesis of antiepileptic drug, (*R*)-lacosamide and its derivative was successfully achieved from known aziridine-(2*R*)-carboxylate in three simple sequential steps including regioselective ring opening of non-activated aziridine, debenzylation followed by acetylation in one pot and amide formation. The advantage of present protocol is that all starting material and reagents are commercially available, single purification by recrystallization after finishing all necessary chemical transformation to yield the final product in >99.9% *ee*.



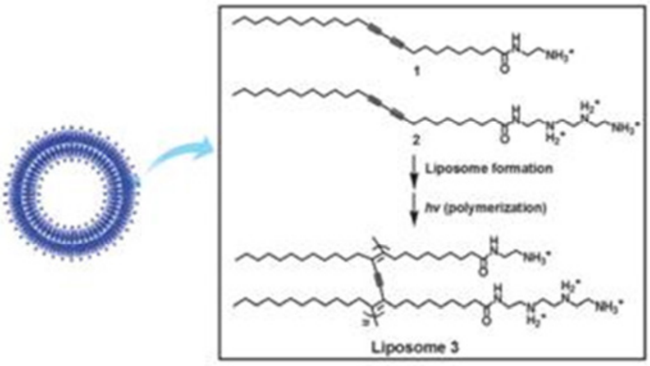
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-271**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Stoichiometric sensing of fatty acids with polydiacetylene liposome

송창욱 안교한*

POSTECH 화학과

Fatty acids play critical roles in biological processes, functioning as a cell membrane component, metabolic responses, inflammatory, energy source and signalling for metabolic regulation.[1] Cis and trans fatty acids have different function in biological processes due to their overall shape. Methods that can selectively sense cis-fatty acids from trans-fatty acids or saturated fatty acids are of significant interest.[2]Herein, we report the polymerized liposome that selectively senses bent fatty acids over linear fatty acids.[3] It has a turn-on type fluorescence change as well as a distinct color change from blue to red. The critical color change was found when two different liposome components contain monoamine and triamine moieties.And also the color change can be correlated with a stoichiometry between the molar ratio of the total liposome components and an analyte cis-fatty acid, oleic acid, in a ratio of 1 : 2.The liposome shows colorimetric response up to the equivalent point with linearity, which enables the monitoring of the content change of cis-fatty acids in commercial cooking oil upon heating at 200 °C.[4]



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-272**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Tumor Targeting Near-Infrared Imaging and Phototherapy Using Cyanine-based Sensor

이다영 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Near Infrared imaging probes are powerful tools for study biological events. Furthermore, the development of theragnostic reagents for specific imaging and therapy have become significant issue. In this study, we synthesized NIR fluorescent probe, CyA-P-CyB for imaging and phototherapy of tumors. CyA-P-CyB have two cyanine moieties via peptide linker which can be cleaved by cathepsin B in tumor cells. Following the cleavage of peptide linker induced by cathepsin B, CyA can show high fluorescence and the phototherapy agent CyB can show strong cytotoxicity to tumor cells We demonstrated its antitumor efficacy from *in vitro* and *in vivo* test.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-273**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Anthradan: a two-photon dye for tissue imaging

박현진 안교한*

POSTECH 화학과

Two-photon microscopy (TPM) is a powerful technique for studying biological systems due to the reduced photo-damage and allowing deeper tissue imaging as it uses longer wavelength light.[1] The donor-acceptor (D–A) type dipolar dyes generally possess high two-photon action cross-section (TPACS) and are promising to develop probes for TPM. Acedan, 6-acetyl-2-(dimethylamino)naphthalene and its analogues are well known dipolar dye and extensively used for TPM.[2] During bioimging, on the contrary, acedan and its analogues suffer from auto-fluorescence interference from the biomolecules because of the overlaps between absorption and emission wavelengths of acedan and that of biomolecules such as riboflavin and flavoproteins. Thus, it is necessary to develop new dipolar dye which can absorb and emit light at longer wavelength. Herein, we introduce a new type of anthradan dye, 9,10-bis(o-dimethoxy-phenyl)-anthradan with absorption and emission wavelength maxima at ~460 nm and ~600 nm respectively, which is within first biological optical window. We also carry out ex vivo imaging experiment for mouse tissues by TPM which results in a bright fluorescence image at internal layer (~25 μm depth), showing negligible fluorescence decrease. Thus the new anthradan dye and its analogues are promising for development of fluorescence probes for bioimaging, especially for deep tissue imaging.References1.a) D. Kim, H. G. Ryu, K. H. Ahn, *Org. Biomol. Chem.* 2014, *12*, 4550-4566; b) H. M. Kim, B. R. Cho, *Chem. Rev.* 2015, *115*, 5014-5055; c) W. R. Zipfel, R. M. Williams, W. W. Webb, *Nat. Biotech.* 2003, *21*, 1369-1377.2.H. M. Kim, B. R. Cho, *Chem-Asian J.* 2011, *6,* 58-69

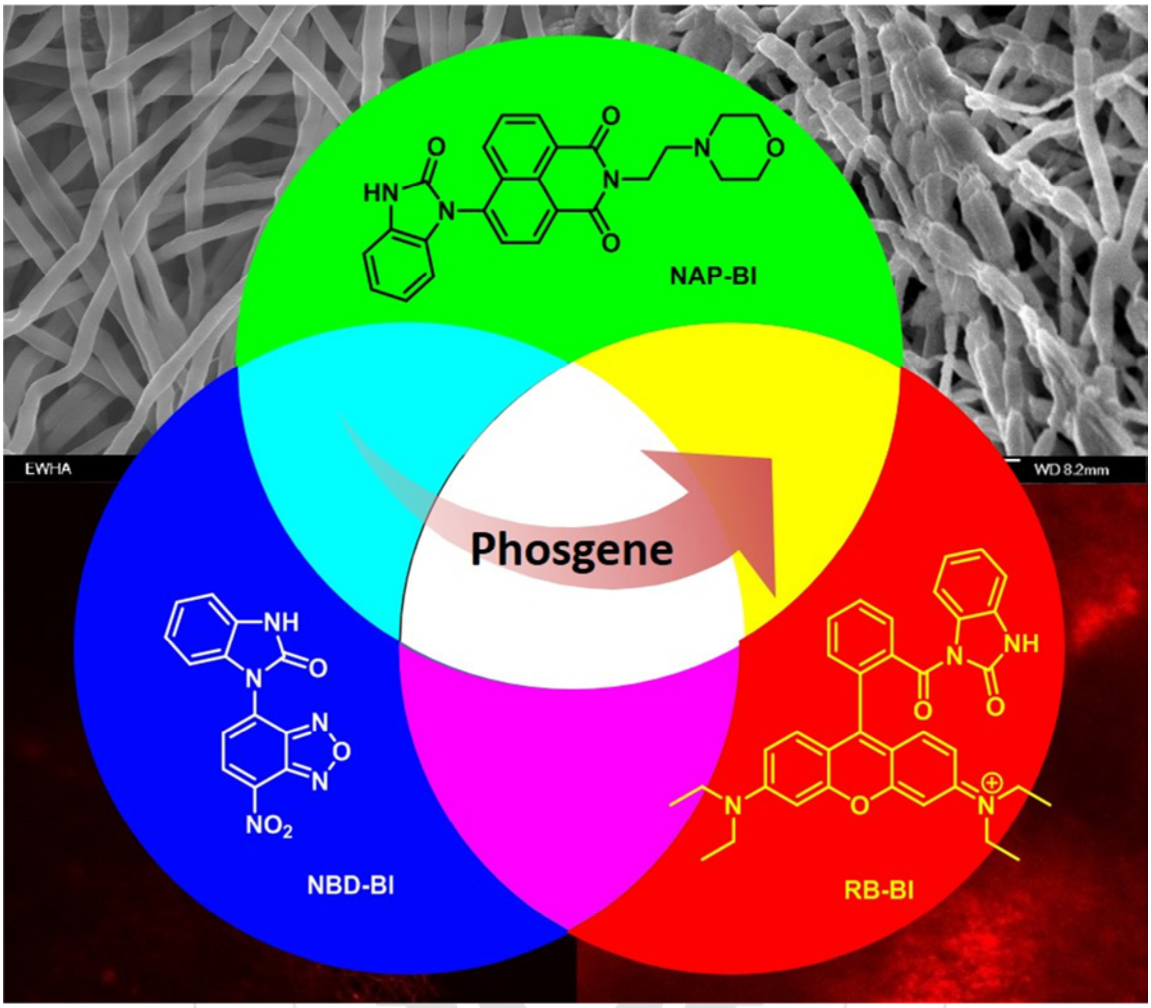
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-274**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Small Organic Dyes and Nanofiber Platforms Based Effective Strategy for Colorimetric and Fluorescence Sensing of Phosgene

Hu Ying CHENLIYAN 김명화[1,*] 윤주영[2,*]

이화여자대학교 화학-나노과학과 [1]이화여자대학교 화학 나노과학과 [2]이화여자대학교 화학·나노과학과

Three different derivatives have been synthesized and utilized as phosgene selective sensors. 4-chloro-7-nitrobenzo[c][1,2,5]oxadiazole (NBD) derivative, rhodamine and naphthalimide were used as representative platforms and either o-phenylenediamine (OPD) was introduced as reacting moiety with phosgene. Unlike previously reported examples, in which chemical reactions converting alcohols or amines to phosphate ester and phosphoramide were utilized, in the current approach, OPD reacts with phosgene to produce corresponding benzimidazolone derivatives via sequential phosphorylation processes. NBD-OPD displayed a distinct UV change as color change from dark orange to pale yellow by naked eye and a fluorescent enhancement with phosgene by the detection limits of 0.7 ppb. On the other hand, the addition of phosgene induced a clear color change from colorless to pink as well as turn-on fluorescent enhancement for RB-OPD via unique spirolactam ring opening process with the detection limit of 2.8 ppb. NAP-OPD also showed turn-on fluorescent enhancements upon the addition of phosgene with the detection limits of 2.8 ppb. Furthermore, NBD-OPD and RB-OPD-embedded polymeric fibers were prepared by electrospinning in order to show distinct colorimetric and fluorescent changes upon the exposure to phosgene under even the solid state.


NAP-BI
NBD-BI
RB-BI
Phosgene
EWHA
WD 8.2mm

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-275**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Total Synthesis of Hericerin Isolated from Hericium erinaceum

문보현 김상용 이윤미*

광운대학교 화학과

Hericium erinaceum is a traditional edible mushroom used as a food and herbal medicine in East Asia. This mushroom shows various biological properties such as antitumor, antioxidant, and many other biological activities. In recent studies, hericerin isolated from Hericium erinaceum has known as a crucial factor for these versatile biological activities. The first synthesis of hericerin was reported by Kobayashi and coworkers in 2012, however, long synthetic steps were required and the overall yield was low. Another method was described by the Miranda group in 2013. Herein we proposed a more efficient approach to hericerin through two key steps: double Mannich type reaction with methyl 4-bromo-3-hydoxy-5-methoxybenzoate and Pd-catalyzed Suzuki coupling reaction. Hericerin was obtained in 45% of improved overall yield through 5 steps.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-276**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fluorescence-based Chemosensors for Histidine Phosphorylation

권오현 최이건[1] 김학진[2] 기정민*

UNIST 화학과 [1]UNIST 나노생명화학공학부 [2]UNIST Chemical Engineering

Post-translational modifications (PTMs) play important roles in regulating the target proteins' functions and physiological outcomes. Phosphorylation is an example of PTMs crucial in cell signaling and metabolism. For example, histidine phosphorylation is found in two component system (TCS), the most popular bacterial signaling system, which functions through the phosphorylation of histidine and aspartate residues. Histidine phosphorylation is also implicated in chromatin remodeling via the phosphorylation of histone H4. However, histidine phosphorylation has not been thoroughly investigated while phosphorylation on serine, threonine and tyrosine has been studied well, because of phosphohistidine's chemical instability and the resultant deficiency of proper research techniques and tools. To address this, we report our progress to develop fluorescence-based chemosensors for histidine phosphorylation. Herein, we report our progress to develop fluorescence-based chemosensors for histidine phosphorylation. Preliminary results in the application to real-time assays of histidine kinases and phosphatases are also presented. Kee, J.-M., Muir, T. W.* "Chasing Phosphohistidine, An Elusive Sibling in the Phosphoamino Acid Family", ACS Chemical Biololgy, 2012, 7, 44-51

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-277**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Cu-catalyzed Electrophilic C-N bond Formation with Alkenylaluminums via Hydroalumination of Internal Alkynes

윤홍주 김유나 이윤미*

광운대학교 화학과

Enamines are significantly synthetic intermediates in organic transformations such as regioselective alkylations or acylations, cycloadditions, and formation of heterocycles. The classical approach for the synthesis of enamines is Lewis acid-catalyzed condensation of a secondary amine with carbonyl group, Buchwald-Hartwig amination using vinyl halide compounds, and various types of transition metal-catalyzed hydroamination of alkynes. Recently, electrophilic amination reactions with vinyl metals for synthesis of enamines have been less reported (e.g. vinylborons and vinylzirconiums). In this study, we focused on the reactivity of aluminum reagents prepared from hydroalumination of internal alkynes with dibal-H for Cu-catalyzed electrophilic amination of O-benzoyl hydroxylamines. The catalytic process is effective and practical to afford the desired enamine products in good to high yields.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-278**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-pot Synthesis of 4-Hydroxy-quinoline Derivatives via Cu-catalyzed Aza-Michael Addition/Cyclization

강성일 김선주 이윤미*

광운대학교 화학과

4-Hydroxy-quinolines constitute one of the important skeletons of numerous alkaloids and synthetic molecules showing interesting biological properties such as BoNT/A LC inhibitors, cancer, and broad-spectrum antibiotic. Although various methods for the synthesis of 4-hydroxy-quinolines have been studied, there are some shortcomings for their synthetic utility. For example, long synthetic steps are required and reactions are carried out under harsh reaction conditions, such as high temperature. Herein, we developed an efficient and mild method for the one-pot synthesis of 4-hydroxy-quinoline derivatives using methyl anthranilates. One-pot cyclization undergoes through Cu-catalyzed aza-Michael addition of methyl anthranilates to vinyl ketones, followed by the treatment of in situ-generated β-amino ketones with KOt-Bu to afford the cyclized quinolinol products. It is noteworthy that the cyclized products can be purified by trituration and recrystallization without column chromatography. A variety of 4-hydroxy-quinoline derivatives are obtained under mild reaction conditions in high yields (up to 98%).

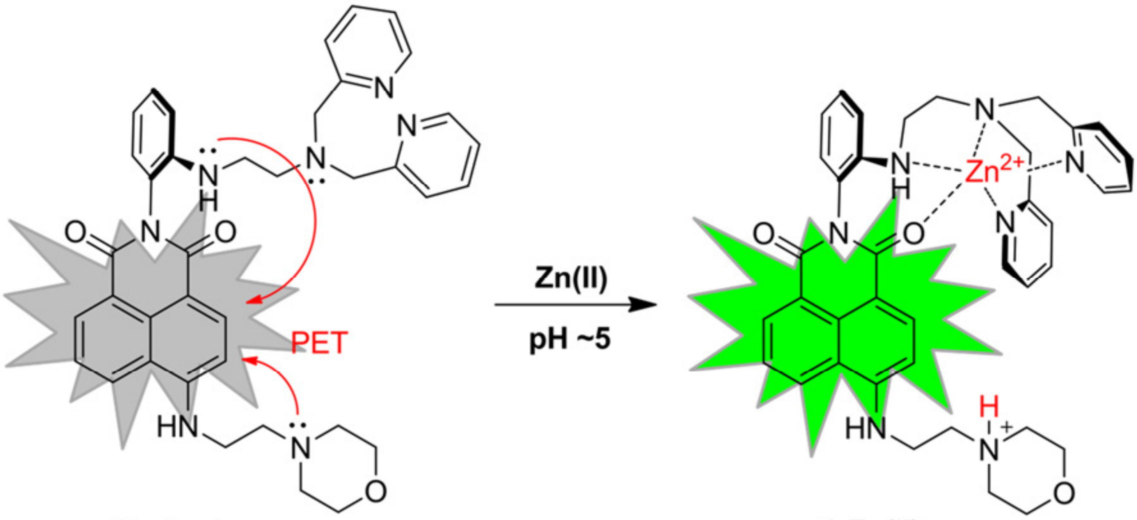
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-279**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Novel Two-Photon Excitable Probe for Zinc Ions in Lysosomes

배주량 안교한[*]

POSTECH 화학과

For maintaining biological functions such as biological redox systems, enzymatic functions, and cellular signalling, Zn(II) is of paramount importance.[1] Influence of Zn(II) on human health has motivated scientists to investigate “Zn(II) biology” by fluorescence methods. Especially development of fluorescent probe which can detects lysosomal Zn(II) ions is necessary for study of oxidative stress levels in biological systems associated with LMP process. Herein, we have developed innovative two-photon probe using naphthalimide dye composed N,N-di-(2-picolyl)ethylenediamine (DPEN) ligand and a morpholine unit. It only fluoresces in the presence of Zn(II) ions at the lysosomal pH (pH 4.5–5.5), with high sensitivity as well as improved selectivity over the most competing Cd(II) ions. The probe can also enabled fluorescence imaging of mouse brain tissues under two-photon excitation at 900 nm. The probe can be a effective tool for studying biological processes related to lysosomal Zn(II) ions by two-photon microscopy.[2]Reference1. (a) C. J. Frederickson, *Int. Rev. Neurobiol.*, 1989, *31*, 145; (b) A. S. Nakashima and R. H. Dyck, *Brain Res. Rev.*, 2009, *59*, 347.2. Lee, H.-J.; Cho, C.-W.; Seo, H.; Singha, S.; Jun, Y. W.; Lee, K.-H.; Jung, Y.; Kim, K.-T.; Park, S.; Bae; S. C.; Ahn, K. H. *Chem. Commun.*, 2016, *52*, 124.



Probe 1 **1-Zn(II)**

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-280**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Direct reductive amination of aldehydes and ketones by Hantzsch ester using N,N'-Diphenyl S-benzyl isothiouronium salt derivatives

이민희 김택현[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 응용화학공학부 광바이오사업단

Direct reductive amination of carbonyl compounds such as aldehydes and ketones is the great method to form Amines. In this reaction, Hantzsch ester is a reductive reagent that can overcome some problems encountered with the traditional reductive reagents. and has biomimic structure. But Hantzsch ester was found to be ineffective without catalyst in some cases. Previously, Thiourea catalysts were the best combinations. Recently S-benzyl isothiouronium has been reported as more effective catalyst which makes N-H parts more acidic than thioreuas accelerating reaction rate. And isothiouronium salts are studying for Direct reductive amination of carbonyl compounds such as aldehydes and ketones in this presentation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-281**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The Gradient Fromation of Surface Chemical Functionalization on Non-biofouling Polymer-Coated Glass surfaces by Surface Organic Chemistry

하은래 오경석 고상원[1] 이정규[*]

경북대학교 화학과 [1]한국철도기술연구원 교통환경연구팀

Surface chemical gradients have recently received a great deal of attention in a variety of research areas because they provide the exceptionally versatile interfaces accessible and develop many technological applications, such as microarrays, molecular discovery, and bio and chemo sensors.1 Surface chemical gradients have allowed for the formation of a gradual variation of chemical functionality on a surface, thereby generating smart materials, understanding surface-driven transport phenomena, and providing quantitative analysis with reliability.2 We herein demonstrate two different methods for the fabrication of surface chemical gradients on non-biofouling polymer coated-surfaces: (i) stoichiometry-based post modification using surface organic reactions and (ii) the controlled adsorption of self-assembled monolayers (SAMs) followed by surface-initiated controlled radical polymerization. In particular, we concentrated on the gradient formation of aldehyde functionality since the aldehyde-amine chemistry has been widely utilized in various research areas.References1. S. Noimark, C. W. Dunnill, M. Wilson, I. P. Parkin, Mater. Horiz. 2014, 1, 322. (a) B. Li, B. Yu, W. T. S. Huck, W. Liu, F. Zhou, J. Am. Chem. Soc. 2013, 3, 317; (b) S. O. Krabbenborg, C. Bicosia, P. Chem, J. Huskens, Nat. Commun. 2013, 4, 1667.

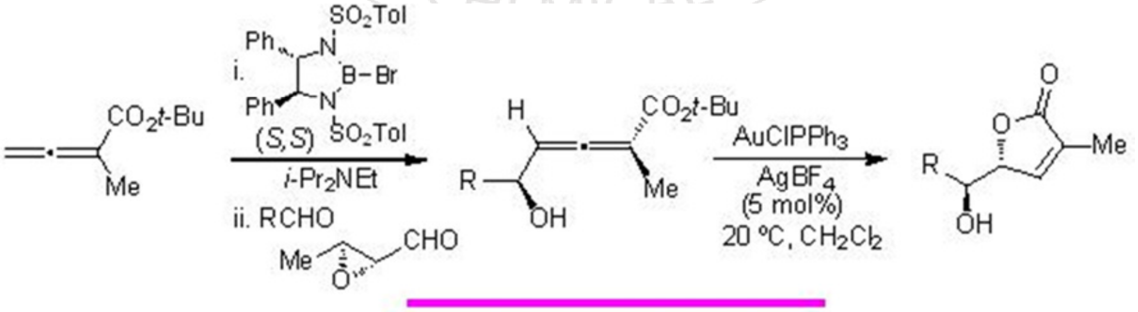
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-282**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

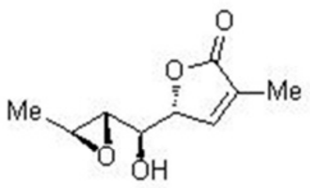
A Highly Regio- and Stereospecific Asymmetric Carbonyl Addition Reaction of Allenoates: Synthetic Applications to Natural Products

이지은 오창화[1] 박새한샘[1] 정희중[1] 김지민[1,*] 유찬모[*]

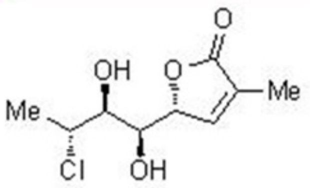
성균관대학교 화학과 [1]전남대학교 화학과

The availability of efficient synthetic methods for achieving absolute stereoselectivity in the production of enantiomerically pure compounds is of considerable current interest because such products can be used as chiral building blocks for the synthesis of valuable chiral substances. Recently, we have developed a new aldol method of the allenoate process in forming 2-hydroxy allenolate in high levels of enantioselectivity. In light of this progress, we turned our attention to achieve unprecedented gamma addition of allenoates to establish center and axial chirality. We would like to present herein the scope of reaction, stereoselectivity, and its applications. We will present regulation factor for reactions and synthetic applications including gold catalyzed cyclization and synthetic studies to (+)-hypoxylactone and xylogiblactone A will also be discussed.

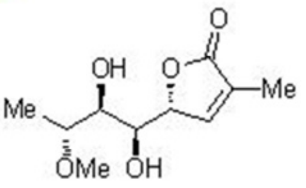




(+)-Hypoxylactone



(+)-Xylogiblactone A



(+)-Xylogiblactone C

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-283**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Zinc Porphyrin-Spiropyran Dyad as Cyanide Sensor

고용민 신은주[1,*]

순천대학교 기초의화학부 [1]순천대학교 화학과

Spiropyran derivatives have been extensively studied as typical photochromic molecules. Spiropyran has also been reported as a selective, sensitive, and reproducible cyanide anion receptor, based on the covalent bond formation between spiropyran and nucleophilic cyanide anion. UV irradiation on coloreless spiropyran with cyanide anion resulted in the formation of yellow-colored merocyanine-cyanide adduct by nucleophilic addition of cyanide anion to merocyanine formed by photochemical ring-opening of spiropyran. Colorless spiropyran was reproduced from merocyanine-cyanide adduct by irradiation with visible light.Metalloporphyrins are intense-colored molecules which show the wavelength shift of Soret absorption band with different ligands. Many metalloporphyrins are useful cyanide sensors because cyanide has high affinity for many metals in metalloporphyrins and also have been used for common anticyanide antidotes for humans.It is expected that the combination of metalloporphyrin and photochromic spiropyran could lead to an interesting light-controllable molecular sensor for cyanide anion. We report here that zinc porphyrin-spiropyran dyad plays a role as a photoresponsive cyanide-selective sensor.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-284**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Detection of Multiple Metal Cations (Co2+, Pb2+, Al3+, In3+) Based on Spiropyran-Isoquinoline Dyad

고용민 신은주[1,*]

순천대학교 기초의화학부 [1]순천대학교 화학과

Spiropyran(SP) are one of the promising families of photochromic compounds with respect to external stimuli such as light, thermal, protons, and metal ions. These stimuli promote reversible heterocyclic cleavage of the spiro C-O bond followed by cis-trans isomerization, producing a metastable merocyanine(MC). A negatively charged phenolic oxygen in the zwitterionic open MC form acts as a chelating site for a variety of metal ions. By functionalizing a photochromic SP with a suitable metal-binding site, light-regulated uptake and release of the metal ion could be possible and thus a regenerable metal-ion sensing system could be constructed. Incorporating isoquinoline ring into SP is expected to lead to excellent light-controlled colorimetric and fluorometric ion sensing system. In this study, a dyad composed of spiropyran and isoquinoline was synthesized and metal cation-sensing ability was examined.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-285**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of higher contents of di-styrenated phenol in addition reaction of styrene with phenol using mixed catalysts in mild condition

김빛나 신은주* 정민철[1] 안호근[1]

순천대학교 화학과 [1]순천대학교 화학공학과

Hydroarylation reaction of styrene with phenol in the presence of catalyst yields the mixture of mono-, di-, and tri-styrenated phenol. Technical mixture of these styrenated phenols is important industrial materials and has been widely used as rubber or plastic stabilizer, antioxidant, and nonionic surfactant, etc. Hydroarylation reaction of styrene or other alkenes with phenol or arenes is one of the most important C-C bond-forming reactions in organic chemistry. These reactions are usually assisted by either protic acid or Lewis acid. However, most of these reactions have some limitations such as the use of large amounts of catalysts, high temperature, strong acidic conditions, low selectivity, moisture sensitivity, high cost, large amounts of waste materials, difficult removal of catalysts, and high toxicity. Therefore, we have investigated to search suitable catalysts for higher contents of di-styrenated phenol in hydroarylation reaction of styrene with phenol in more mild condition. Some mixed catalysts are superior to single catalyst and make hydroarylation reaction to occur even in room temperature.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-286**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Colorful Bioorthogonal Turn-on Probes with a Single Fluorescent Core Skeleton

이영준 김은하[1] 박승범*

서울대학교 화학부 [1]아주대학교 분자과학기술학과

Recently, tetrazine(tz)-alkene ligation has received great attention in the field of chemical biology as a robust bioorthogonal reaction. A noticeable feature of this reaction is ultrafast kinetics between tetrazines and strained alkenes through the Inverse Electron Demand Diels-Alder reaction (IEDDA). On top of that, in terms of spectroscopy, tetrazine was known as a potential fluorescence quencher when conjugated with fluorophores, and abolished its quenching ability after transformed into pyridazine via the reaction with alkenes. Taking these into consideration, the tetrazine-based fluorophore can be a useful turn-on probe for rapid and specific visualization of the biological objects.Seoul-Fluor(SF) is a unique fluorophore whose fluorescent emission and the quantum yield can be predictably modulated by changing its functional groups. We envisioned the tetrazine-based Seoul-Fluor(Tz-SF) to generate the colorful bioorthogonal turn-on probes in a facile manner. Two different versions of the Tz-SF system will be presented, one is direct pi-system conjunction between the SF and the Tz, and the other is aliphatic linker type conjunction. The detailed results will be discussed in the poster section.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-287**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation and Spectroscopic Properties of Spiropyran-Pyrene Dyad

류경아 신은주[1,*]

순천대학교 기초의화학부 [1]순천대학교 화학과

Click reactions has commonly found in organic synthesis. Triazole-conjugated spiropyran-pyrene dyad was synthesized by copper catalyzed alkyne-azide click reaction between spiropyran containing propargyl group and pyrene containing N_3 group. 2,3,3-Trimethylindolenine underwent propargylation with 1-tosyl-2-propyne to afford 1-propargyl-2,3,3-trimethyleneindoline. Condensation reaction of 1-propargyl-2,3,3-trimethyleneindoline with 2-hydroxy-5-nitrobenzaldehyde resulted propargyl-substituted spiropyran, SP-C≡CH. Pyrene-OTs was obtained by the reaction of pyrene-OH and tosyl chloride, TsCl. Azide-functionalized pyrene, Py-N_3 was prepared from the reaction of pyrene-OTs and NaN_3 . Triazole-conjugated spiropyran-pyrene dyad as a form of 1,4-disubstituted 1,2,3-triazole was synthesized using click reaction between SP-C≡CH and Py-N_3 , Spectroscopic properties of spiropyran-pyrene dyad were investigated with absorption and fluorescence spectroscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-288**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Gold-catalyzed hydroarylation of styrene with phenol

양현영 김빛나[1] 신은주[1,*] 정민철[2] 안호근[2]

순천대학교 기초의화학부 [1]순천대학교 화학과 [2]순천대학교 화학공학과

Intermolecular hydroarylation of styrene with phenol has been accomplished with various acid catalysts to give mixture of styrenated phenol. Technical mixture of styrenated phenol contains mono-, di-, and tri-styrenated phenol. In this work, the reaction was catalyzed by Gold(Ⅲ). Hydroarylation reaction of styrene with phenol was carried out with AuCl3 catalyst. To optimize the reaction conditions with AuCl3 catalyst, reactions were studied under the various reaction conditions such as styrene/phenol mole ratio, solvent, reaction temperature, reaction time, AuCl3/phenol mole ratio, and so on.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-289**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of β-Amino Sulfones through Cu-Catalyzed Aza-Michael Reaction of (Hetero)aryl Amines to Vinyl Sulfones

김성철 강성일 이윤미*

광운대학교 화학과

β-Amino sulfone compounds containing a aromatic amine or aromatic aza-heterocycle substituent are an important building block for preparation of natural products, medicines, and functional materials. Although numerous methods for synthesis of β-amino sulfone compounds have been studied, aza-Michael addition is one of the simplest reactions and 100% atom economy reaction. Traditionally, aza-Michael additions were performed under strongly acidic or basic conditions, but, these reactions have some problems; the need for high reaction temperature and long reaction times. Transition-metal catalyzed aza-Michael addition has emerged as a powerful tool for an efficient and mild synthesis of β-amino compounds. In this study, we described an efficient and mild Cu catalyst system for aza-Michael addition of a variety of aromatic amines or aza-heterocycles to vinyl sulfones. The inexpensive Cu salt, readily available phosphine or imidazolium salts, and KOt-Bu were used to generate a Cu-amido complex in situ as the catalytic species. A wide range of β-amino sulfones bearing aniline, indole, carbazole, pyrrole, imidazole, pyrazole, and triazole derivatives were obtained in up to 99% yield in the presence of 3−7 mol % copper complex at ambient temperature.

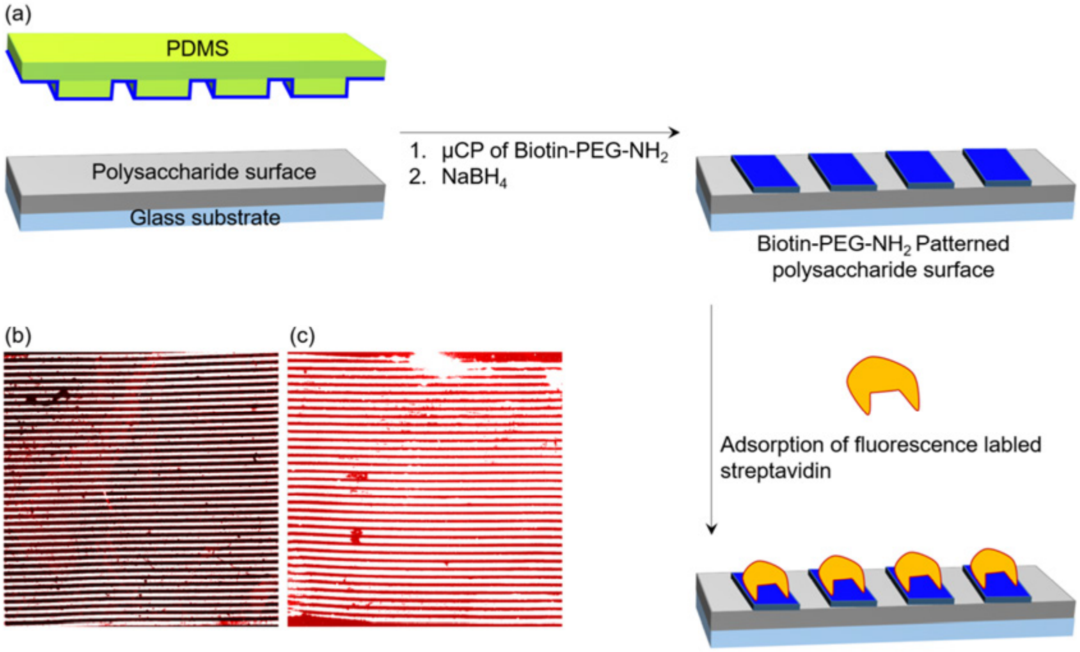
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-290**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Systematic Investigation of Non-Biofouling Polysaccharide Films on a Large-Area Glass surface with Microcontact Printin

한경엽 김형욱 고상원[1] 이정규*

경북대학교 화학과 [1]한국철도기술연구원 교통환경연구팀

Biofouling, the deterioration of device and surface function resulting from the accumulation of biological matter (i.e., proteins, cells, and microorganisms), is an important issue in a wide range of fields, including biosensors, biomedical devices, medical implants, marine equipment, water purification, and drug delivery carriers.1 Thus, it is necessary to introduce functionalities on solid surfaces, which minimize the unwanted, non-specific adsorption of bioentities as well as improve the device function.2-7 Conventional research showed micrometer-sized patterning, and was thus difficult to apply it for practical applications. To overcome this drawback, we, herein, demonstrate biopatterning on a large-area (1 cm × 1 cm) polysaccharide films using microcontact printing technique. In particular, we carefully monitored how much the polymer thickness affected the non-biofouling efficacy using biotin-streptavidin as a model study. With a fluorescence scanner, we successfully compared the signal-to-noise ratio and the binding capacity as the thickness of the polymeric film was changed.References1. S. Noimark, C. W. Dunnill, M. Wilson, I. P. Parkin, Chem. Soc. Rev. 2009, 38, 34352. S. Jiang, Z. Q. Cao, Adv. Mater. 2010, 22, 920.3. J. K. Lee et al., Chem. Asian J. 2015, 10, 568. 4. W. K. Cho, S. M. Kang, J. K. Lee, J. Nanosci. Nanotechnol. 2014, 14, 1231.5. S. P. Jeong, D. Hong, S. M. Kang, I. S. Choi, J. K. Lee, Asian J. Org. Chem. 2013, 2, 568.6. S. P. Jeong, B. S. Lee, S. M. Kang, S. Ko, I. S. Choi, J. K. Lee, Chem. Comm. 2014, 50, 52917. S. P. Jeong, S. M. Kang, D. Hong, H.-Y. Lee, I. S. Choi, S. Ko, J. K. Lee, J. Nanosci. Nanotechnol. 2015, 15, 1767.


(a)
PDMS
Polysaccharide surface
Glass substrate
1. μCP of Biotin-PEG-NH_2
2. $NaBH_4$
Biotin-PEG-NH_2 Patterned polysaccharide surface
Adsorption of fluorescence labled streptavidin
(b)
(c)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-291**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Biomimetic nucleophilic catalysts based on neighboring group effects

정호영 오주영 안승민[1] 김학진[2] 기정민[*]

UNIST 화학과 [1]UNIST 자연과학부-화학 [2]UNIST Chemical Engineering

Formation and hydrolysis of carboxyl derivatives such as ester, thioester and amide are of great importance in organic chemistry. Efficient and specific formation of the amide bond between peptide/protein fragments is critically important for the synthesis of peptides and proteins, with potential impact in many areas including protein drug discovery and bioconjugation. Native chemical ligation is one of such reaction between thioester and an N-terminal cysteine. Despite its exquisite specificity, this reaction is often very slow and requires high concentration of peptides and proteins. Thus thiol-based nucleophilic catalysts are typically employed. Although the catalyst accelerates the reaction by converting the reactant into a more reactive thioester, the reaction is often still slow for many practical applications. To address this, we propose biomimetic nucleophilic catalysts. Introduction of hydrogen donor and acceptor as neighboring groups to nucleophilic catalysts can stabilize the tetrahedral intermediate of acyl substitution reaction. Alternatively, they can activate the nucleophile or the leaving group. In fact, such a mechanism is well known for many enzymes such as proteases and ligases, which dramatically accelerate acyl substitutions under mild conditions. We report our progress on the development of such biomimetic nucleophilic catalyst. These catalysts can have significant impact in the peptide synthesis, bioconjugation, and the development of artificial enzyme mimics.

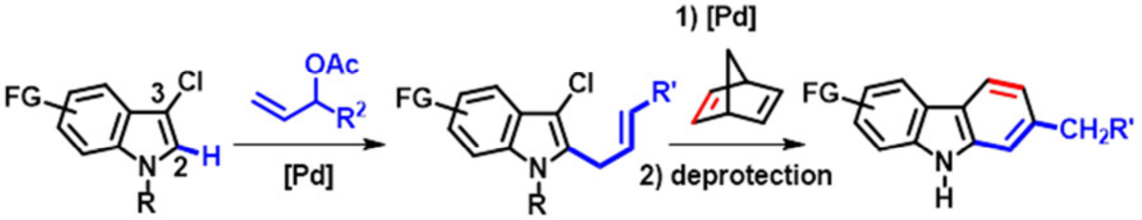
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-292**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Pd-catalyzed C2-allylation of Indoles and Annulation with Norbornadiene for the Synthesis of Carbazoles

이주영 하혜리 한인혁 주정민*

부산대학교 화학과

We have developed a Pd-catalyzed C2-allylation of indoles and subsequent cyclization of the allylated indoles. The electronic effect of chloro and ester groups that can be readily installed at the C3 position of indoles facilitated highly efficient C–H allylation at the C2 position. The resulting 2-allyl-3-chloroindoles were found to be suitable substrates for benzannulation reactions using alkynes and norbornadiene as an acetylene synthon. This approach, utilizing readily available indoles, allyl acetates, and norbornadiene, allows rapid access to complex carbazoles.Reference1. Lee, J. Y.; Ha, H.; Bae, S.; Han, I.; Joo, J. M. Adv. Syn. Catal. (DOI 10.1002/adsc.201600568).



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-293**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Spiro[imidazolidine-4,11'-indeno[1,2-b]quinoxaline]-hydantoins and Schiff base of indeno[1,2-b]quinoxalin-11-ones

신하윤 정대일* 송주현 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Indeno[1,2-b]quinoxaline-11-ones are useful building blocks found in a wide range of biologically active compounds. Moreover, carbonyl group of indeno[1,2-b]quinoxaline-11-ones can further be modified to pharmacologically important functional groups such as hydantoin ring or Schiff base. Hydantoins are found in several medicinally important compounds such as phenytoin and fosphenytoin, anticonvulsants used in the treatment of seizure disorders. Schiff bases are reported to possess a broad spectrum of medicinal and pharmacological activities such as anticonvulsant, antiinflammatory, analgesic and antimicrobial. In this study, a series of indeno[1,2-b]quinoxaline-11-one derivatives are synthesized by the condensation between ninhydrin and various aromatic diamines. A reasonable sequence of events is the addition to carbonyl, substitution of hydroxyl and two elimination of water. Resulting indeno[1,2-b]quinoxaline-11-one derivatives were further modified to form hydantoins and Schiff bases. Hydantoins are obtained by the condensation of potassium cyanide and ammonium carbonate with ketones. Schiff bases are formed by the reaction between compounds with primary amino group and indeno[1,2-b]quinoxaline-11-one derivatives.

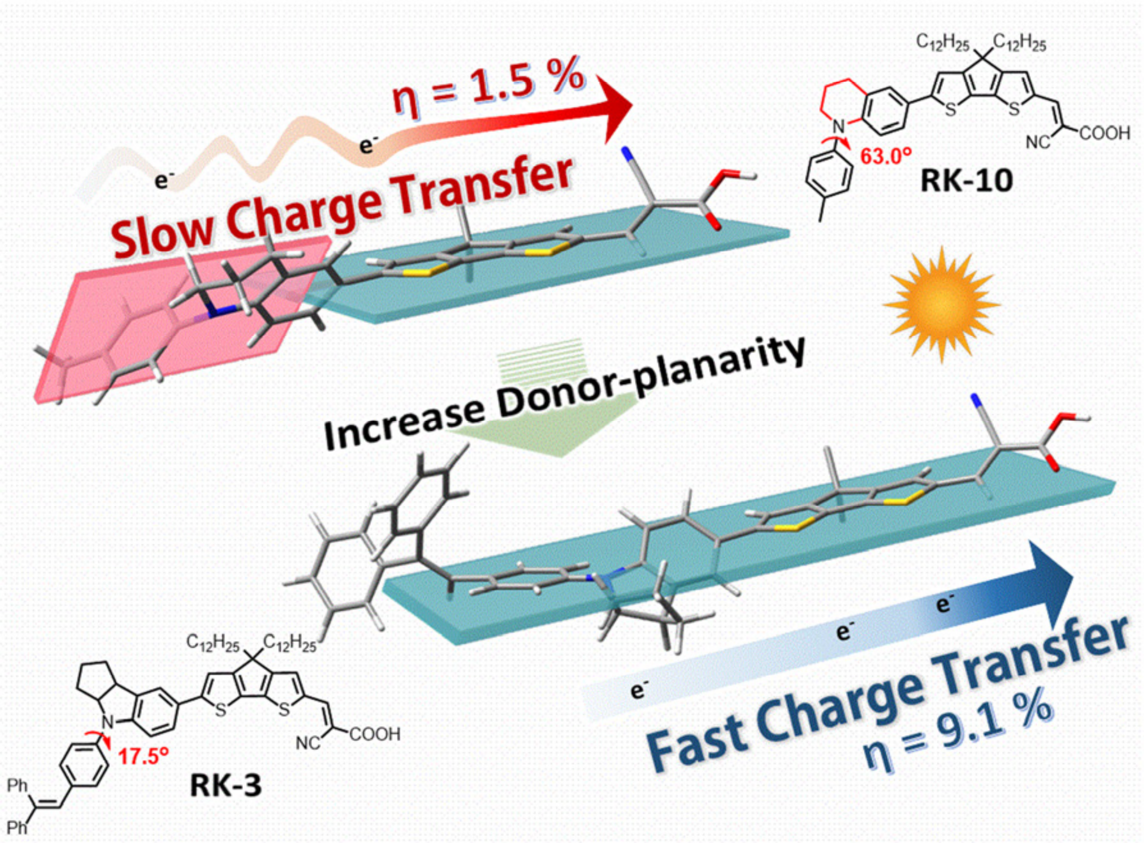
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-294**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Planarity Effect of Indoline-based Sensitizers on Charge Transfer in Thin Film Photoelectrode

박준혁 노덕호[1] 권태혁[2,*]

UNIST 자연과학부 [1]UNIST 화학과 [2]UNIST 친환경에너지 공학부

Molecular engineering for targeting the thin photoanode is important to apply flexible device, solid-state DSC and low-cost fabrications. In addition, it benefits the electrolyte diffusion and lower the charge recombination possibility at TiO2/electrolyte interface. Our team developed organic dye sensitizers targeting thin photoanode, and reported the molecular charge transfer depend on different donors, which have higher molar extinction coefficient and small electrochemical differences, but differ degree of donor-planarity. RK-series dyes, which composed substituted. cyclopentadithiophene as a π linker, we present four new dyes designed with indoline or tetrahydroquinolines moiety as donor. Depending on donors, especially for planarity trend, performances of the device are dramatically changed although relatively smaller change of light-harvesting efficiency. More planar donor dyes, the higher efficiency than non-planar dyes because of their faster charge transfer. In addition, additional donating group on indoline unit, such as RK-3 dye, gives broad light harvesting and retarding recombination effects, which in turn, it reachess the best photo conversion efficiency of 9.1% at the thin films (< 2 μm) with iodine-based electrolyte under 1 sun irradiance of 100 mWcm-2.In this research, we showed the importance of planarity of the donors in Intermolecular Charge Transfer (ICT). Density Functional Theory computation, Time-correlated single photon counting techniques and Impedance spectroscopy were applied to analysis the difference of charge transfer of the sensitizers. Planar donors was successfully investigated, facile charge injection, charge regeneration compared to non-planar donors. As result, D-D planar donor moiety achieved excellent PCE in thin photoanode films.


η = 1.5 %
e⁻
e⁻
Slow Charge Transfer
C12H25
C12H25
N
S
S
NC
COOH
63.0°
RK-10
Increase Donor-planarity
C12H25
C12H25
N
S
S
NC
COOH
17.5°
RK-3
Ph
Ph
e⁻
e⁻
e⁻
Fast Charge Transfer
η = 9.1 %

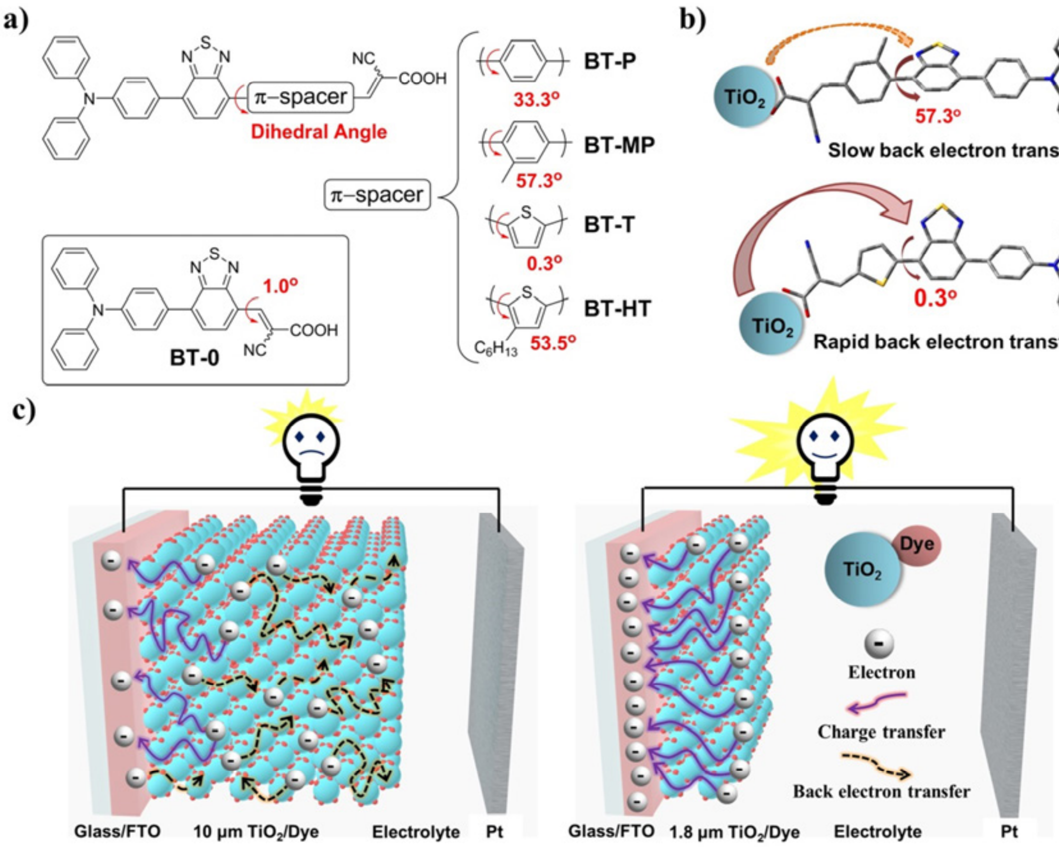
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-295**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Strategy for Improved Photo Conversion Efficiency in Thin Photoelectrode Films by Controlling π-Spacer Dihedral Angle

노덕호 권태혁[1,*]

UNIST 화학과 [1]UNIST 친환경에너지 공학부

Benzo[c][1,2,5]thiadiazole (BT) has been used in dye-sensitized solar cells (DSCs) for its light-harvesting abilities. However, as a strongly electron deficient unit, BT causes rapid back electron transfer (BET), which in turn lowers the power conversion efficiency of devices. Herein, we report a powerful strategy for retarding the effect of BET by controlling both the photoelectrode thickness and π-spacer dihedral angle. To achieve this, we introduced planar (BT-T) or twisted π-spacers (BT-P, BT-MP, and BT-HT) between BT units and anchoring groups, and used different photoelectrode thicknesses between 1.8 and 10 μm. Computational and experimental results show that twisted π-spacers were more efficient at retarding BET than the planar π-spacer. However, BET was found to be less important than expected, and light harvesting efficiency (LHE) played a critical role as the thickness of the photoelectrode decreased because charge collection efficiency was enhanced. The planar dye BT-T obtained the highest LHE, this value remained unusually high even in 1.8 μm photoelectrodes. As a result, BT-T gave a power conversion efficiency (PCE) of 6.5% (Jsc = 13.56 mA/cm2, Voc = 0.67 V and FF = 0.72) in thin 1.8 μm photoelectrodes with 3.5 μm scattering layers, which represented a roughly 40% enhancement compared to the PCE in 10 μm photoelectrodes (4.76%). Overall, these results provide a novel approach to achieving ultrathin and highly efficient flexible DSCs.


a)
N
S
N
N
NC
COOH
π−spacer
Dihedral Angle
BT-P
33.3°
BT-MP
57.3°
π−spacer
S
BT-T
0.3°
S
BT-HT
C_6H_{13}
53.5°
N
S
N
N
1.0°
COOH
NC
BT-0
b)
TiO_2
57.3°
Slow back electron transfer
TiO_2
0.3°
Rapid back electron transfer
c)
Glass/FTO
10 μm TiO_2/Dye
Electrolyte
Pt
TiO_2
Dye
Electron
Charge transfer
Back electron transfer
Glass/FTO
1.8 μm TiO_2/Dye
Electrolyte
Pt

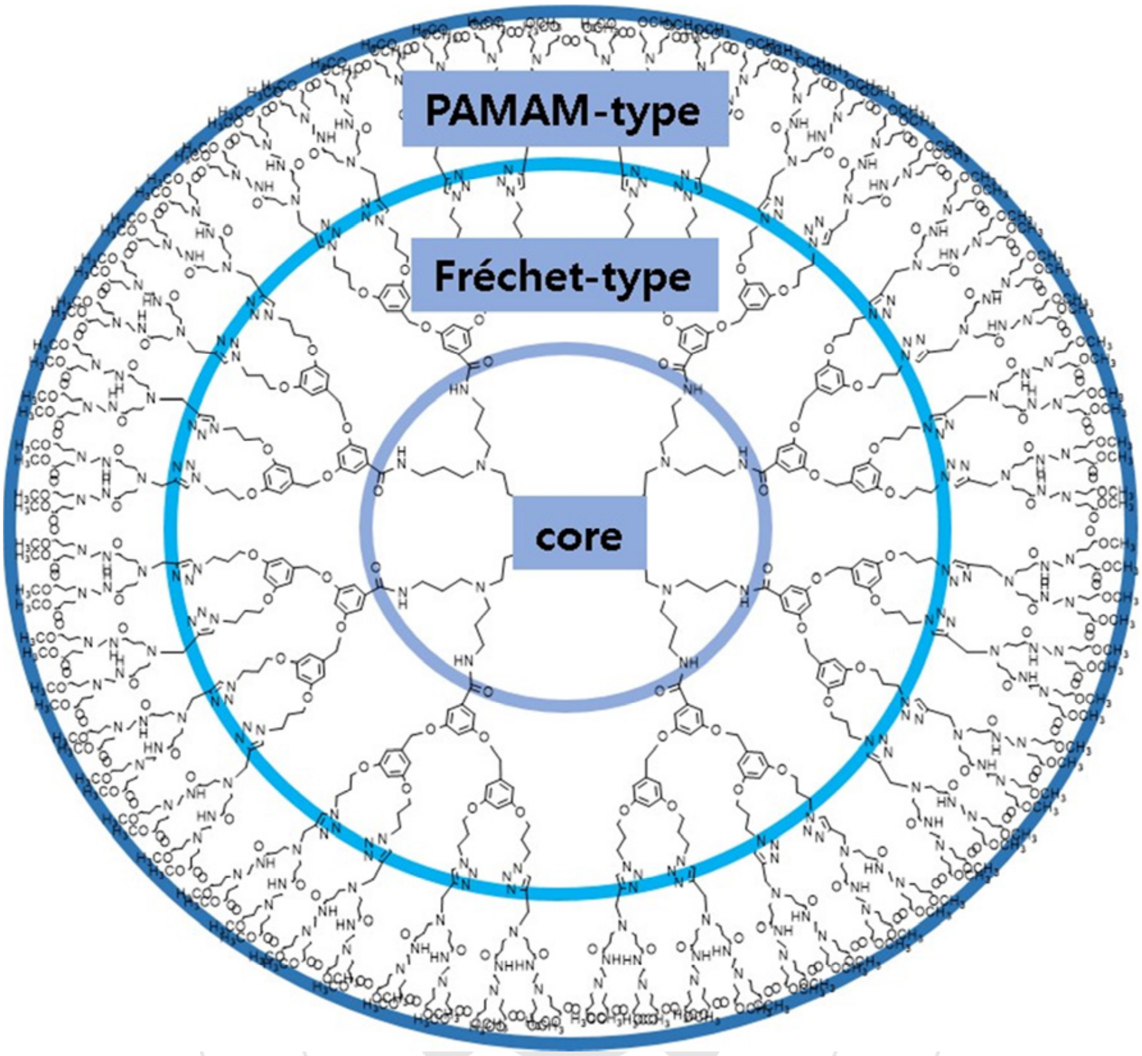
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-296**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Layered Dendrimers via Click Chemistry Using DAB-Am-4,8 Core

도우미 이재욱*

동아대학교 화학과

The click chemistry, which is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition, proved to be an ideal reaction that used as the most practical and reliable chemical transformations and has found in many applications in organic chemistry and synthesis of dendrimer. Taking advantage of these facts, herein we present the efficient strategy for the synthesis of layered dendrimers containing the Fréchet-type polyether block unit and the PAMAM(polyamidoamine)-type block unit having the polypropylene imine(PPI) unit at core region. All dendrimer are characterized by NMR, IR, and Mass analysis.


PAMAM-type
Fréchet-type
core

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-297**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Electrogenerated Chemiluminescence Chemodosimetric Sensing Systems for Sulfide Based on Cyclometalated Ir(III) Complexes

김서연 김훈준 홍종인*

서울대학교 화학부

Electrogenerated chemiluminescence (ECL) is the generation of light from the electron-transfer reaction between electrochemically generated radical species at the electrodes. ECL method has attracted significant attention because ECL technique does not require the use of complex and expensive light sources. Therefore, it provides simple and miniaturized sensing tools. Because of the absence of background optical signal from light sources, ECL can have better detection limit than conventional photoluminescence methods. These features make ECL a highly sensitive and selective analytical method.We designed new ECL chemodosimetric sulfide sensors based on cyclometalated Ir(III) complexes. Some Ir(III) complexes are known as good ECL luminophores because they exhibit tunable luminescent colors at various wavelengths by modulating main ligands. Among them, (piq)2Ir(pic) (piq = phenylisoquinoline, pic = picolinate) exhibits efficient orange-red ECL around 606 nm with TPrA in air-saturated condition. We developed two ECL chemodosimetric probes, based on Ir(III) complexes using piq as a main ligand and pic as an ancillary ligand, for the detection of sulfide anion. While complex 1 shows a low turn-on ratio, complex 2 shows a low phosphorescence of its own due to the additional quenching groups on main ligands. Therefore it provides high turn-on ratio for sulfide anion over the other thiol species. As a result, complex 2 is a good “turn-on” ECL sensor. Details of synthesis, photophysical and electrochemical studies will be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-298**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and fluorescence properties of coumarin aldehyde containing crown ether

박성호 장승현*

대구대학교 화학과

In this research, we synthesized fluorescence sensors from coumarin and benzo crown ethers. The synthetic routes for coumarin containing benzo crown ether were outlined at scheme 1. Two derivatives were synthesized for Schiff base reaction. Thereafter, the structures of the new compounds were confirmed by Melting point, ^{1}H-NMR and GC-Mass. The compounds were found to selectivity about Na^+ and K^+ by fluorescence titration using various metal cations.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-299**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Dendrimers via Homo-coupling of terminal alkyne dendrons using palladium catalyst

우수근 이재욱*

동아대학교 화학과

Palladium-catalyzed cross-coupling reactions are widely used to the formation of C-C bonds. The formation of the alkynyl cuprate, by base-assisted deprotonation of in the presence of CuI, and subsequent transmetalation with Pd(II), gives a dialkynyl palladium(II) species. Final reductive elimination generates Pd(0) and diyne. The Pd(0) species is reoxidized to Pd(II) with various oxidants to complete the catalytic cycle. Alkyne dimerization, through oxidative homo-coupling, to give 1,3-diynes is important for a number of applications, particularly in the construction of linearly π-conjugated acetylenic oligomers and polymers. We are pay attention to this fact to investigate the synthetic method of dendrimer using the alkyne focal dendrons. The alkyne focal fréchet-type dendrons are synthesized by N-alkylation and Staudinger/aza-Wittig reactions. Synthesis of PAMAM-type dendrons is carried out using N-alkylation and Michael reaction. Two different types of denderimers, fréchet-type and PAMAM-type dendrimers, are synthesized by the coupling reaction of terminal alkynes using palladium catalyst. All dendrimers are characterized by NMR, IR, Mass spectrometry, UV-Vis, PL and GPC analysis.

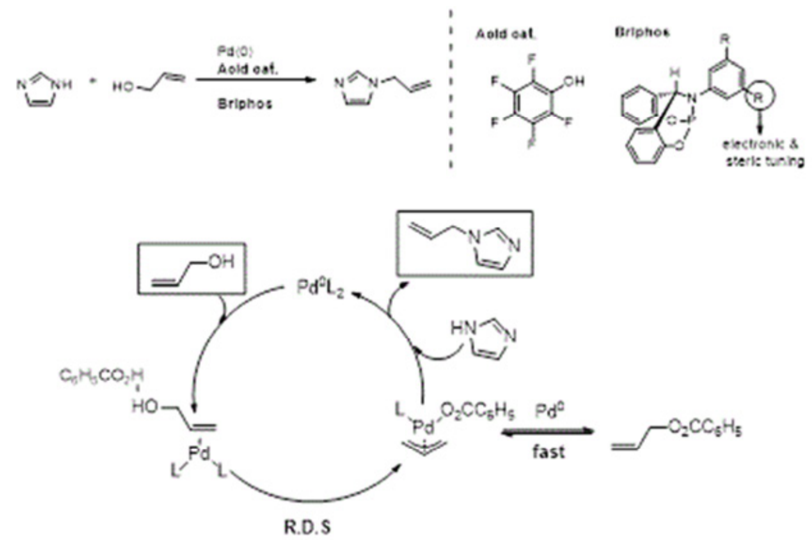
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-300**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dehydrative Direct Cross-Coupling of Allylic Alcohols and N-Heterocycles Promoted by Palladium-Briphos and Acidc Additive

강경준 김현우*

KAIST 화학과

It has been reported that the reactivity and selectivity of transition-metal catalysts can be modulated by the choice of ligands such as phosphorus and N-heterocyclic carbene ligands. Thus, the ligand design is one of major topics in transition metal catalysis. For that purpose, we recently reported bicyclic bridgehead phosphoramidites (briphos) as a new type of π-acceptor ligand.1 Compared with their linear analogues such as monophos, briphos ligands show enhanced π-acceptor ability induced by geometrical constraints. In addition, briphos allows for facile steric and electronic tuning because of their simple and practical synthetic procedures. Here, we explored Pd-catalyzed allylations by using briphos ligands. Pd-catalyzed allylic substitution with allyl alcohols is attractive because only a stoichiometric amount of water can be produced as a by-product. However, the utilization of allyl alcohols is only limited to good nucleophiles such as malonates, alkyl amines, and anilines.2 Moreover, Pd-catalyzed substitution reactions of allylic alcohols with poor nucleophiles such as imidazoles and benzimidazoles are rarely reported.3 Herein, we report an efficient Pd-catalyzed allylation of allyl alcohols with a variety of N-heterocycles facilitated by a π-acceptor ligand, briphos, in a tandem catalytic cycle.


Pd(0)
Acid cat.
Briphos
Acid cat.
F
OH
Briphos
R
H
N
O
P
R
electronic &
steric tuning
OH
Pd^0L_2
N
N
HN
N
$C_6H_5CO_2H$
HO
Pd
L
L
L
Pd
$O_2CC_6H_5$
Pd^0
fast
$O_2CC_6H_5$
R.D.S

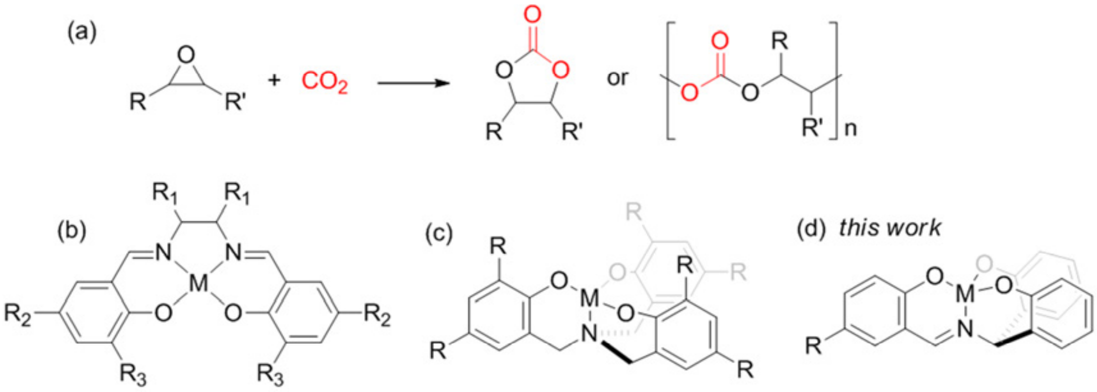
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-301**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Selective Synthesis of Cyclic Carbonates from CO_2 and Internal Epoxides Catalyzed by Fe(Ⅲ)-Catalysts

이유섭 김진 이윤호* 김현우*

KAIST 화학과

CO_2 is an attractive C1 building block because it is abundant and renewable. Also, it is considered as a phosgene replacement due to its nontoxic nature.[1] Therefore, various kinds of CO_2 utilization methods have been developed[2] not only because of these prominent features but also concerns of global warming, since CO_2 is one of green house gases. One of the promising CO_2 utilization method is to make cyclic carbonates from epoxides. Cyclic carbonates are used as polar aprotic solvent, electrolytes or intermediates for organic synthesis. Several catalysts for cyclic carbonates have been reported, including organocatalysts and transition metal complexes. Among them, the properties of salen-based catalysts are quite remarkable, which can switch the selectivity between cyclic carbonates and polycarbonates depending on metal center and ligand structure[3]. Recently, Kleij have reported[4] highly active and selective catalysts for cyclic carbonates with mononuclear Al and dinuclear Fe complexes based on amino tris(phenolate) ligands. According to the DFT computation, authors proposed a transition state where two oxygen atoms each from epoxide and CO_2 bind to the metal center in a cis fashion, thereby greatly lowering the activation barrier.[5] Thus, highly active and selective catalysts for cyclic carbonate synthesis can be developed on the basis of three fold symmetric amino tris(phenolate) ligand scaffolds. We have designed a new class of NO3 ligand for selective synthesis of cyclic carbonates resulting from available cis-binding site of the metal center. Here we introduce highly efficient and selective Fe catalysts based on our C_s symmetric NO3 ligands for coupling of CO_2 and epoxides.



M(salen)

[polycarbonate & cyclic carbonate]

M-**2** (M = Al and Fe)

[cyclic carbonate]

M-**1** (M = Al and Fe)

[cyclic carbonate with internal epoxide]

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-302**

발표분야: 유기화학

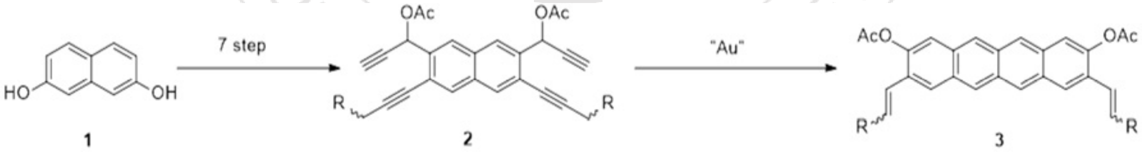
발표종류: 포스터, 발표일시: 금 11:00~12:30

Gold Catalyzed intramolecular Ene-type Reactions to tetracene Derivatives

정재문 오창호* 허훈구

한양대학교 화학과

We reported Au-catalyzed activation of a propargyl acetate, followed by ene-type reaction with a pendant triple bond to provide a variety of 2-acetoxynaphthalene derivatives. This reaction has been extended to syntheses of highly functionalized 2,9-diacetate tetraacenes. First, we prepared model substrates 2 in a 7 step sequence starting from 1, 2,7-dihydroxynaphthalene. Then we studied their cyclization under gold catalysis. We wish to report our preliminary results concerning the syntheses and physical properties of the tetracenes like 3



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-303**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Perylene based probes for sensing of electron rich salicylic acid derivatives in EtOH

Anup Pandith 김홍석*

경북대학교 응용화학과

Recently aminopropylimidazole units were incorporated with various fluorophores such as anthracene and pyrene for highly selective sensing of electron deficient phenolic and salicylic acid derivatives. Further to explore the importance of secondary amine and imidazole unit through propyl spacer, we extended our work and successfully implemented with perylene as probes 1, 2 and 3. Designed probe 1 showed extensively high association constant towards electron rich salicylic acid (SA's) derivatives in a 1:1 binding stoichiometry than the electron deficient counterparts in absolute ethanol. Higher selectivity towards electron rich SA's derivatives attributed due to the synergistic multiple hydrogen bonding, π-π and non-classical NH-π interactions between probe 1 and electron rich SA's derivatives.

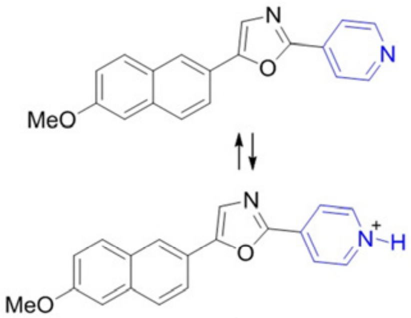
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-304**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Syntheses of Fluorescent probe based on Fluorene and naphthalene skeletons

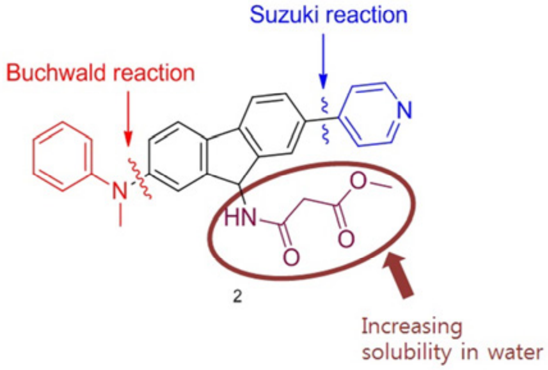
이태희 박희정[1] 박균하[2,*]

한국화학연구원 화학분석센터 [1]한국기초과학지원연구원 서울서부센터 [2]충남대학교 화학과

pH Probe which can visualize pH levels in normal and cancer tissues were synthesized. For the purpose, naphthalene and fluorene skeletons have been adopted as the fluorophore reporter. Syntheses of the two probes were prepared starting with 2-acetyl-6-methoxynaphthalene and fluorene. we have used $CuBr_2$ to induce selective α-bromination followed by reacting with hexamethylenetetramine(HMTA) to introduce amino functionality, finally to afford 2-[2-(4-pyridinyl)-5-oxazolyl]-6-methoxynaphthalene and 2-(N-methyl-N-phenyl)amino-7-(4-pyridinyl)-[3-(methyl 3-oxopropanoate)amino]-9H-fluorene will be discussed. The structures of synthesized compounds were identified using IR, NMR, LC-MS and elemental analyses.



1



2

Increasing solubility in water

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-305**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dual selective fluorescence detection of Al(III) and fluoride ions with an “off-on-off” switch

임치섭 허준혁[1] 김홍석[*]

경북대학교 응용화학과 [1]경북대학교 응용화학

A simple 2-(2’-hydroxyphenyl)-4-formyl-thiazole based probe (HAT, 1) was designed and synthesized. Probe 1 selectively detected Al(III) with a fluorescence enhancement, and sequentially 1-Al ensemble detected fluoride ions selectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-306**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Capsule-pseudorotaxane type of hybrid supramolecular assembly based on cavitand and copillar[5]arene

유선호 송규민 박도혜 박연실 백경수*

숭실대학교 화학과

Hybrid supramolecular cavitand 1 easily forms a stable molecular capsule in the presence of p-disubstituted benzene guests(G_1) such as 1,4-diiodobenzene or 1,4-dimethoxybenzene. Molecular capsule $G_1@1_2$ is stabilized by eight intermolecular -N-H•••O=C(amide part) hydrogen bonds. Capsule-pseudorotaxane is formed by cation-π interactions between imidazolium cationic guests (G_2) and 8 copillar[5]arene parts of $G_1@1_2$. This hybrid supramolecular assembly was confirmed by 1H-NMR, 2D-ROESY, 2D-DOSY NMR and mass spectroscopy.

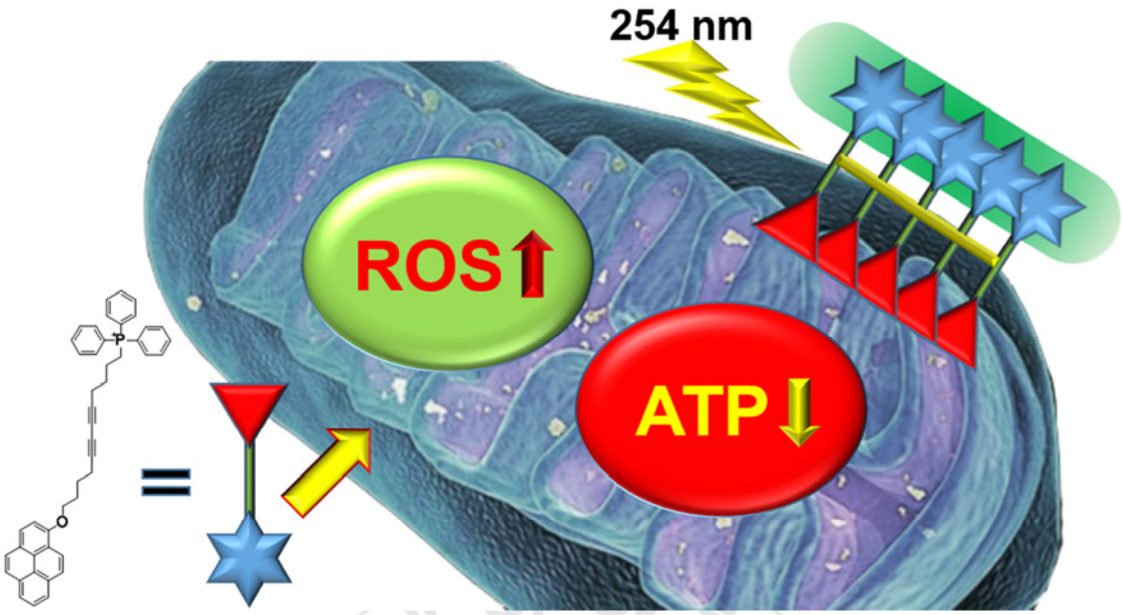
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-307**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Phosphonium-diacetylene-pyrane conjugate controlling mitochondria activity

이재홍 이용재 김태우* 강철훈*

경희대학교 동서의학대학원

Subcellular organelle-specific reagents for imaging and treatment are of enormous interest in mitochondria activity. herein, we designed, synthesized and present a mitochondria targeting probe (TPP-ACE-Py) by conjugating a triphenylphosphine (TPP) with a fluorogen which can undergo pyrene excimer. The mitochondria targeting probe (TPP-ACE-Py), the presence of Triphenylphosphonium (TPP) group specifically guide the mitochondria. Upon irradiation of light (by a 254 nm UV Lamp), the diacetylene(ACE) group of photo polymerization, resulting in a bathochromic shift of the fluorescent wavelength (from 375 and 398 nm for the monomer) to a longer wavelength (550 nm for the excimer) and is able to quickly and selectively polymerization in mitochondria.The probe polymerization in mitochondria was found to decrease the mitochondrial activity and induce the generation of ROS.


254 nm
ROS
ATP

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-308**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Syntheses and biological evaluation of analogues of Acinetobactin for iron acquisition

정다와 송운영 이민욱 김학중*

고려대학교 화학과

Iron is essential for the survival of all forms of life, in which it involves in key metabolic processes. However, due to the low aqueous solubility of Fe(III), all organisms possess dedicated systems to actively assimilate the iron from the aerobic environment. Siderophores are small organic molecules utilized by bacteria for Fe(III) acquisition by chelation Fe(III) from the outside. Acinetobacter baumannii, one of the most notorious Gram-negative pathogens, secretes several siderophores including acinetobactin. Acinetobactin contains three potential metal-chelating motifs; catechol, hydroxamate, and imidazole. Initially, its structure was reported to have an oxazoline ring, but later it turned out to be rearranged to an isoxazolidinone. Although its structure including potential ligands and feature that two possible forms exist via isomerization revealed, little is known about the binding mode with Fe(III). In the presented study, we designed and synthesized ten acinetobactin analogues having modified chelating ligands. The synthesis was successfully completed by slight modifications of the synthetic route for acinetobactin that we have established. Then, various analytical experiments and cell growth promotion assays were conducted to prove proper ligands for iron acquisition and physiological siderophore form between two isomers.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-309**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Naphtoimidazolium Cholesterol as Fluorescent Chemosensors for Chiral Recognitions with Amino Acid

고경주 윤주영[1,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학·나노과학과

Chirality plays an important role in biochemical systems. The majority of organic substances from all living creatures are chiral molecules. Enantiomers often have very different physiological properties. For example, D-amino acids are generally sweet whereas the L-amino acids are bitter or tasteless. Therefore, chiral recognition is of great significance in chemistry and biochemistry. Various techniques have been used for the chiral recognition, such as NMR, UV/vis, and fluorescence spectroscopy. Chiral fluorescence sensors allow for rapid determination of the enantiometric composition of chiral compounds with high sensitivity. We synthesized naphtoimidazolium cholesterol receptor as chiral and fluorescent hosts for the recognition of amino acids. Naphtoimidazolium cholesterol was examined for their chiral recognitions with D- and L-t-Boc-amino acid anions, such as alanine(Ala), Phenyl alanine(Phe), Tartaric acid(Tart), Threonine(Thr), etc.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-310**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Catalytic Activities of Functionalized Titanium(IV) Molecular Clusters

김수연 김영익 김영조 김민[*]

충북대학교 화학과

Titanium is an earth abundant early transition metal, and very useful element for catalysis (including photo-catalysis) and material science. In the concept of catalysis for organic reactions, it is known that titanium(IV) could be utilized to various interesting organic transformations such as Diels-Alder reaction, 1,2- or 1,4-additions, and Lewis acid-mediated reactions.[1-3]

In addition, titanium is also applied to various organic/inorganic hybrid material synthesis including metal-organic frameworks (MOFs) or porous molecular clusters. Due to the high oxophilic character of titanium ion and strong interaction between titanium and carboxylate group, it is known that titanium-carboxylate MOFs and molecular clusters are generally stable than other transition metal clusters. At the same time, the strong interaction between titanium(IV) and carboxylate prevents the organic functionalization of titanium-MOFs or titanium molecular clusters. Recently, Chun group reported practical synthesis of titanium(IV) molecular clusters and it was reported that this titanium(IV) molecular clusters selectively absorb CO_2 with high capacities. However, only alkyl- and amino(NH_2)-group functionalized titanium(IV) clusters were successfully synthesized from the solvothermal condition.[4,5]

In this presentation, we will discuss about the catalytic activities of titanium(IV) molecular clusters to cycloaddition of CO_2 and photo-catalytic degradation of organic molecules. The preparation of titanium(IV) molecular clusters and their structure analysis along with the functional group tolerances in the titanium(IV) molecular clusters will be presented.

References

[1] Yus, M.; Ramón, D. J. *Chem. Rev.* **2006**, *106*, 2126.

[2] Teets, T. S.; Maity, A.; *Chem. Rev.* **2016**, *116*, 8873.

[3] Bahnemann, D. W.; Schneider, J.; Matsuoka, M.; Takeuchi, M.; Zhang, J.; Horiuchi, Y.; Anpo, M.

Chem. Rev. **2014** , *114*, 9919.

[4] Hong, K.; Chun, H. *Inorg. Chem.* **2013**, *52*, 9705.

[5] Hong, K.; Bak, W.; Chun, H. *Inorg. Chem.* **2014**, *53*, 7288.

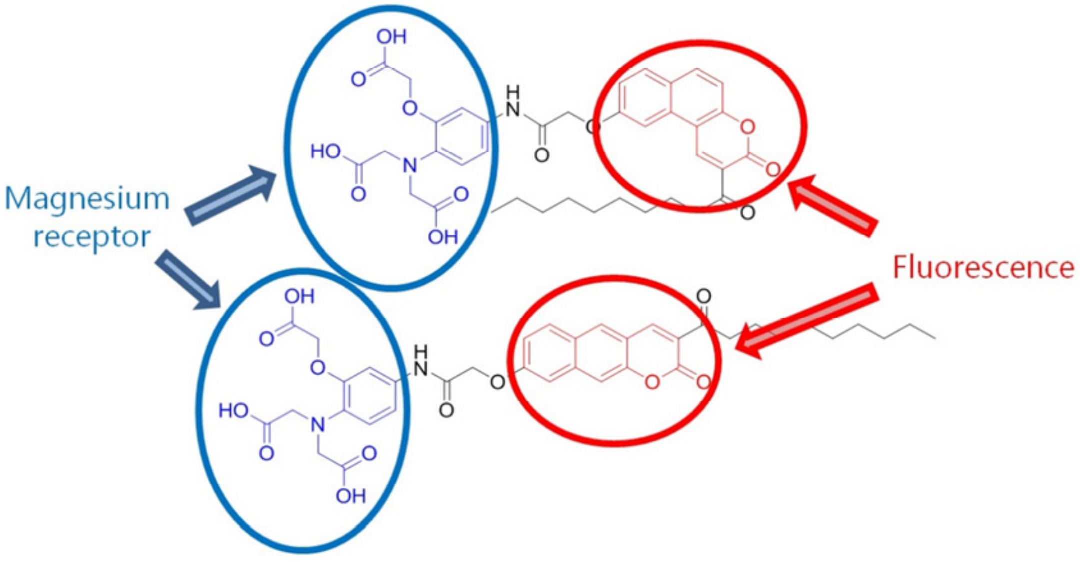
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-311**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Syntheses of fluorescent metal probe of regiosisomeric coumarins

이태희 박희정[1] 박균하[2,*]

한국화학연구원 화학분석센터 [1]한국기초과학지원연구원 서울서부센터 [2]충남대학교 화학과

Coumarin fluoreophores have been utilized to metal probes. Herein two kinds of regioisomeric coumarins were synthesized starting form 2.7-dimethoxynaphthalene. we will discuss the syntheses of two regioisomeric coumarins by following different synthetic processes. The structures of synthesized compounds were identified using IR, NMR, LC-MS and elemental analyses.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-312**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of a cell-based screening system for inhibitor of Amyloid-β by a fluorescent unnatural amino acid

이태진 양승현 김주환 강효진 정상전*

동국대학교 화학과

Aggregation of the amyloid-β peptide is one of the key factors leading to Alzheimer's Disease (AD).[1] A myriad of evidence suggest that the formation of amyloid-β aggregates is greatly influence by high concentrations of metal (II) ions.[2] We designed a fast and reliable detection system based on Förster resonance energy transfer (FRET) technology to image amyloid-β aggregation using an amyloid-β fluorescent probe. In this system, the tryptophan (λ_{Ex} = 280 nm, λ_{Em} = 330 nm) residue in amyloid-β serves as the FRET donor. Naphthylamine (λ_{Ex} = 330 nm, λ_{Em} = 430 nm) was selected as the FRET acceptor and was conjugated to the side chain of an aspartic acid residue by an amide bond. Previously, metal-ion induced amyloid-β aggregation was detected *in vitro* using FRET and TEM (Transmission Electron Microscopy). However, the use of the aspartic acid-naphthylamine conjugate hampers the exploitation of the developed system in a cell based assay. Cell based assay requires the expression of the amyloid-β probe using the orthogonal tRNA/synthetase pair that is able to incorporate an unnatural amino acid. Recently, a synthase that is able to use unnatural amino acids as substrates was identified. This synthase recognizes a 'carbamate bond' contrary to the amide bond used previously. Therefore, we synthesized Naphthyl-ε-Lysine having a carbamate bond to use in cell based assays. In the future, the amyloid-β FRET probe including the unnatural amino acid will be expressed in cell for inhibitor assay of amyloid-β.(1)Estrada, L. D. Journal of Alzheimer's disease : JAD 2016.(2)Tiiman, A. Journal of Alzheimer's disease : JAD 2016.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

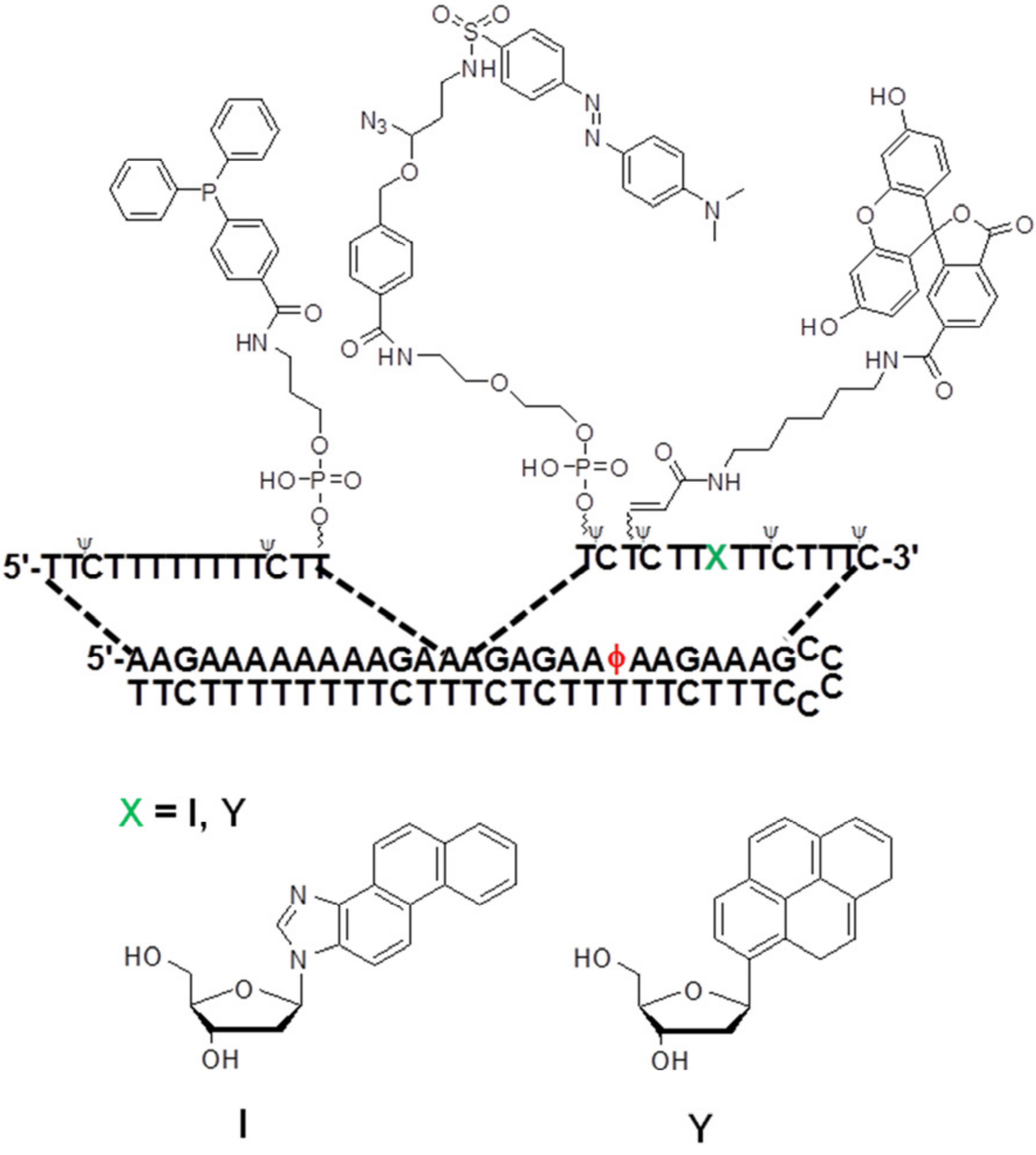
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-313**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Templated chemistry for monitoring damage and repair directly in duplex DNA

김보연 이성호*

대구대학교 화학응용화학과

We report the fluorogenic detection of the product of base excision repair (an abasic site) in a specific sequence of duplex DNA. This is achieved by DNA-templated chemistry, employing triple helix-forming probes that contain unnatural nucleobases designed to selectively recognize the site of a missing base. Light-up signals of up to 36-fold were documented, and probes could be used to monitor enzymatic removal of a damaged base.



ϕ = abasic or THF (undamaged = A)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-314**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Photo-Reactive Fc Binding Peptide-NODA Conjugates for Imaging of Rheumatoid Arthritis

이사묵 김주환 강효진 정상전*

동국대학교 화학과

Rheumatoid arthritis (RA) is a progressive autoimmune disease leading to chronic inflammation of the joints, particularly the hands. RA patients suffer from cartilage and bone deformations eventually causing immobility of the limbs. Risk factors associated with the development of RA include TNF-α, IL-1, IL-6, and IL levels, which are key infiltrates in inflamed subsynovium and proinflammatory cytokines. TNF-α is known to be one of main regulators of the immune response and a viable target in the treatment of RA. Traditionally, well-known methods for diagnosing and managing early onset of RA involve the use of conventional radiography, ultrasonography, and magnetic resonance imaging. In our approach, a photo-reactive Fc binding peptide (FcBP) is used to selectively target and covalently bind the Fc-domain of Enbrel, a biopharmaceutical antibody fusion protein that inhibits TNF-α. Furthermore, the radio isotope carrier, 1,4,7-triazacyclononane-diacetic acid (NODA), is covalently attached to the photo-reactive FcBP. Previously, it was demonstrated that FcBP is a very convenient tool to immobilize functional materials to the Fc-region of antibodies in a reversible and site-specific manner1. The synthesized FcBP-NODA complex possess strong chelating properties and high selectivity towards di- or trivalent metals2. Our developed complex enables RA imaging by radio isotope. Successful development of this RA diagnosing tool may find application in RA cell imaging as well as in the monitoring of drug delivery. 1. Y. Jung, H. J. Kang, J. M. Lee, S. O. Jung, W. S. Yun, S. J Chung, and B. H. Chung, Anal. Biochem., 374, 99 (2008)2. Yongkang Gai, Zhongping Hu, Zhao Rong, Xiang Ma * and Guangya Xiang, molecules 19393-19405, 20 (2015)

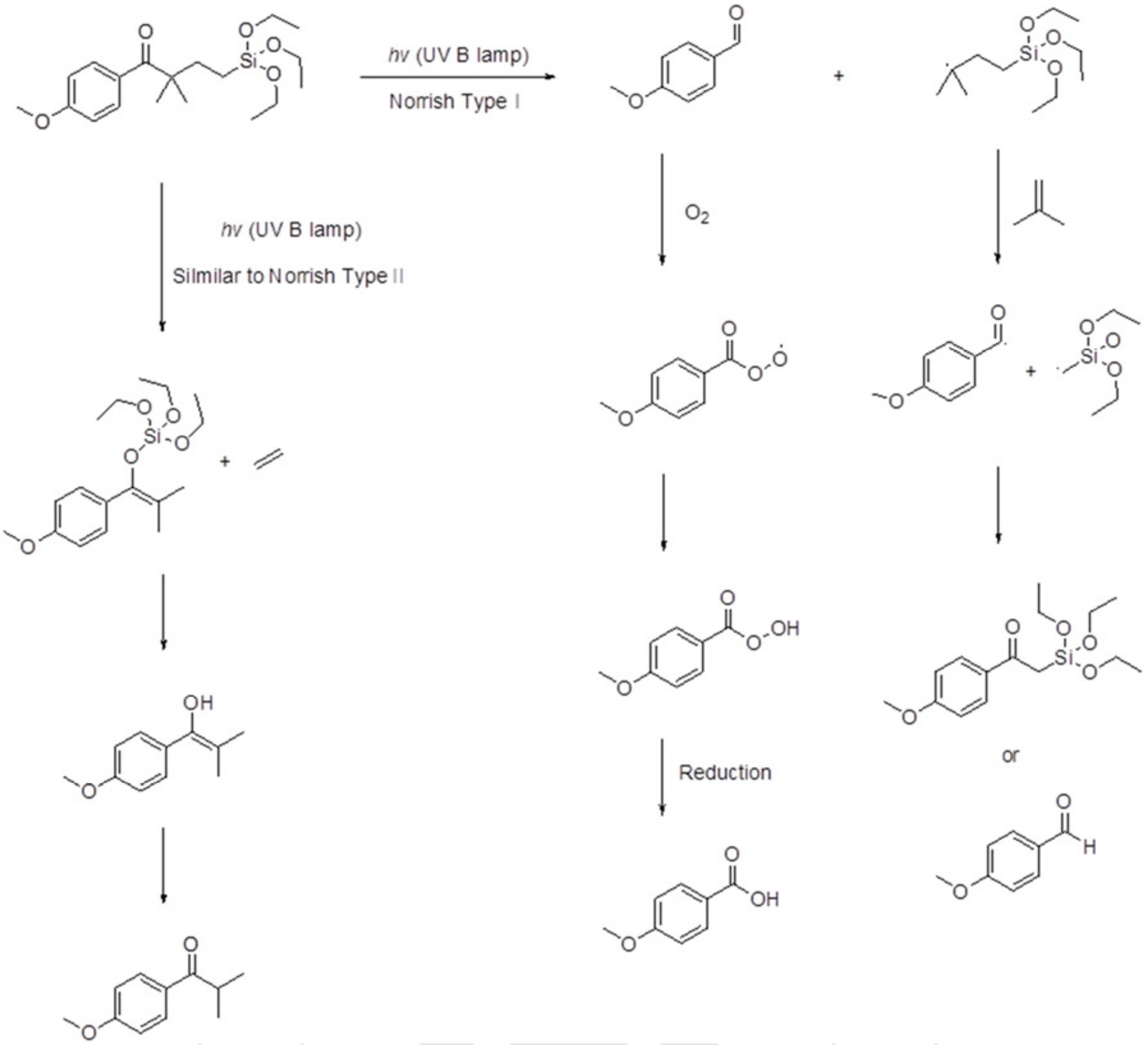
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-315**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Study of benzoyl group photocleavage in a trialkoxysilane system

전가영 문봉진*

서강대학교 화학과

Photochemical reaction can occur by absorption of photons with ultraviolet (wavelength from 100 - 400 nm), visible light (400 - 750 nm) or infrared radiation (750 - 2500 nm). In organic chemistry, eletrocyclic reaction, radical reaction, photoisomerization and Norrish reaction are representative photochemical reactions. Among them, Norrish reaction takes place with aldehyde or ketone. The reaction is generally classified into type I and type II. An adhesive is a material used to bind two surfaces together. The adhesive works by van der Waals interaction, hydrogen bonding, and covalent bond. In our research was desired an adhesive that can adhere to a surface by chemical interaction but can be cleaved by a stimulus such as UV-irradiation. To test the viability of the idea, benzoyl group that can absorb UV light was introduced to a trialkoxysilane and its photochemical behavior was investigated. Once UV B was applied onto the synthesized material, α bond of benzoyl group was homolytically cleaved, and two free radical intermediates were formed. This reaction is called Norrish Type I. In another type of reaction, trialkoxysilyl group on γ position was transferred to carbonyl oxygen and 1,4-radicals was formed by internal photochemical reaction. This reaction is similar to Norrish Type II.1 The generated radicals produced variable compounds through many pathways. From GC-MS data, it was observed that the product of Norrish Type I and II reaction as well as several other byproducts were formed.


hv (UV B lamp)
Norrish Type I
+
hv (UV B lamp)
Silmilar to Norrish Type II
+
O2
+
Reduction
or

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-316**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ring-Opening of Cyclic Peptoids

김정윤 권용억*

이화여자대학교 화학.나노과학과

Peptoids (N-substituted oligoglycines) where alkyl side chains are attached to amide backbone nitrogens are useful synthetic peptidomimetics. Major advantages of peptoids as chemical tools for chemical biology and drug development include the ease synthesis, high variation of each unit, resistance to proteolytic degradation, and interesting biological activities. Especially, cyclic peptoids have been in the spotlight for their improved cell permeability, higher proteolytic resistance, and stronger binding affinity against specific proteins. In our previous studies, we have reported the several strategies for the development of cyclic peptoids and the unusual truncation of acylated peptoids under acidic conditions. The main problem of cyclic peptoids as chemical tools for screening studies is that it is very difficult to sequence the hit compounds by common methods such as tandem mass spectrometry or Edman degradation. In this presentation, we report a robust platform for the site-specific opening of macrolactamized cyclic peptoids, followed by tandem mass spectrometry-based sequencing strategy.

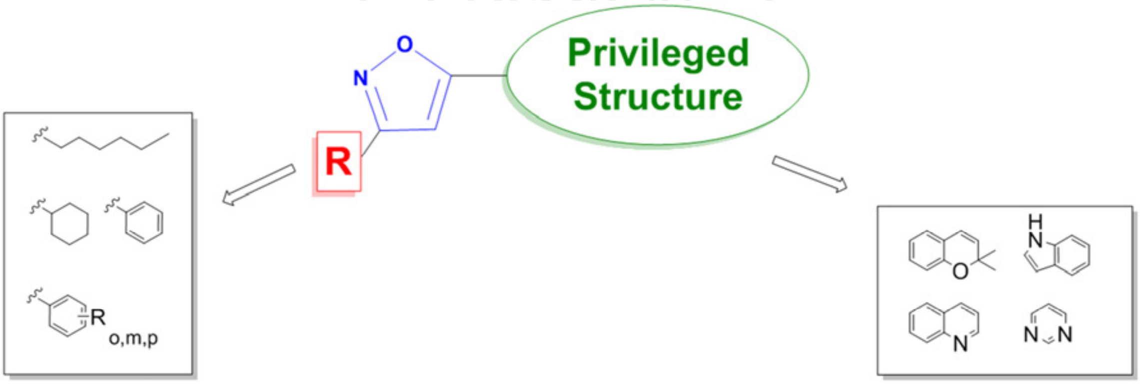
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-317**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Library Construction of the 3,5-Disubstituted Isoxazole with Diverse Substituents and Privileged Structures

황윤수 김민지 박승범*

서울대학교 화학부

Isoxazole is a five-membered aromatic heterocycle containing nitrogen and oxygen in a 1,2-relationship. Its two electronegative heteroatoms can engage in hydrogen bond donor/acceptor interactions with a variety of enzymes and receptors which can increase the potential of desired pharmacological activities.We designed the isoxazole with two strategies. One is introduction of diverse substituents on one side of the core which can provide rooms for structure-activity relationship study and further modification. The other is introduction of privileged structures, which have high biological relevancy, on the other side. We constructed the isoxazole core using 1,3-dipolar cycloaddition as a synthetic strategy. In a combinatorial manner, 90 compounds were easily synthesized and we will apply our library to some biological experiments. We expect that our library would show some novel or improved biological effects.



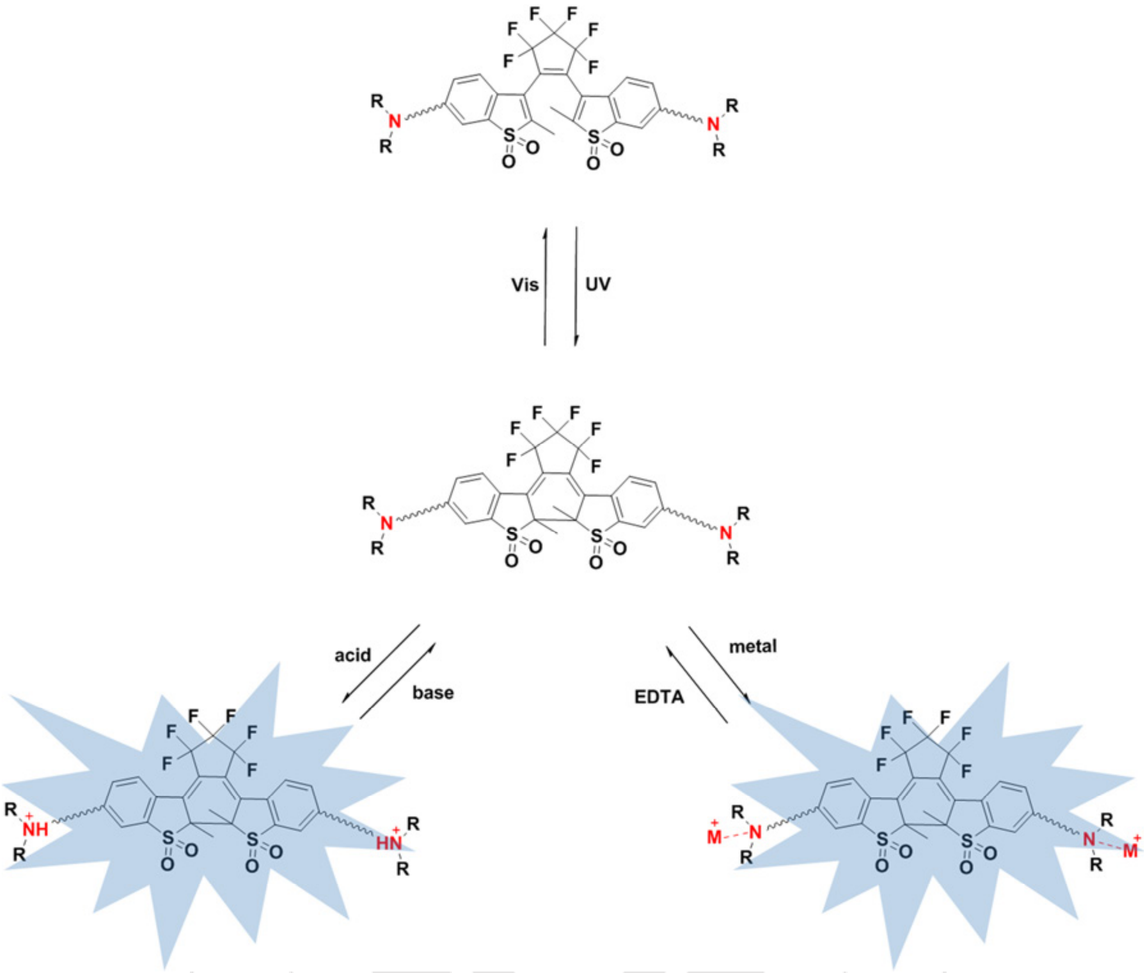
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-318**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Photochromic PET acid/metal sensor

류지경 윤호준 안광현[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Photochromic diarylethenes have been widely utilized for the construction of photoswitchable systems because of their excellent thermal stability and outstanding fatigue resistance. To prepare photoswitchable PET sensors, the fluorescence “turn-on” diarylethenes was linked to the fluorescent acid or metal ion sensors, so that the fluorescence intensity can be modulated via the photoisomerization of the photochromic moiety. Strong fluorescence was observed for the closed form of the diarylethenes with acid or metal ion, and the emission intensity was up to four times higher than initial closed form.


Vis
UV
acid
base
metal
EDTA

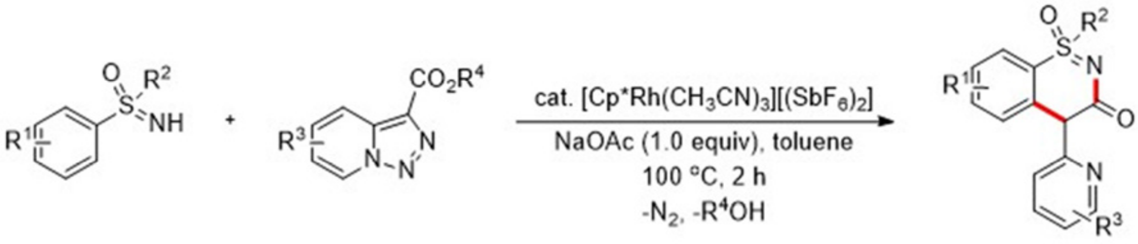
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-319**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rh-Catalyzed C-H Activation/Cyclization/Elimination from *S*-Aryl Sulfoximines and Pyridotriazoles for the Synthesis of 1,2-Benzothiazines

김종혜 손정유 이필호*

강원대학교 화학과

Sulfoximines are novel privileged scaffolds that have been applied as pharmaceuticals and bioactive compounds as well as ligands and chiral auxiliaries in asymmetric syntheses. As a consequence, the development of efficient methods for the synthesis of sulfoximines and their functionalizations is greatly needed. However, despite the significant advances made in the functionalization of sulfoximines, only a few examples of 1,2-benzothiazines, which are more attractive pharmacophores as a type of cyclic sulfoximine, have been reported. Herein, we have developed an efficient synthetic method for a wide range of 1,2-benzothiazines bearing pyridyl as well as carbonyl groups by a rhodium-catalyzed domino C−H activation/cyclization/elimination of alcohol process starting from *S*-aryl sulfoximine and pyridotriazole compounds.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



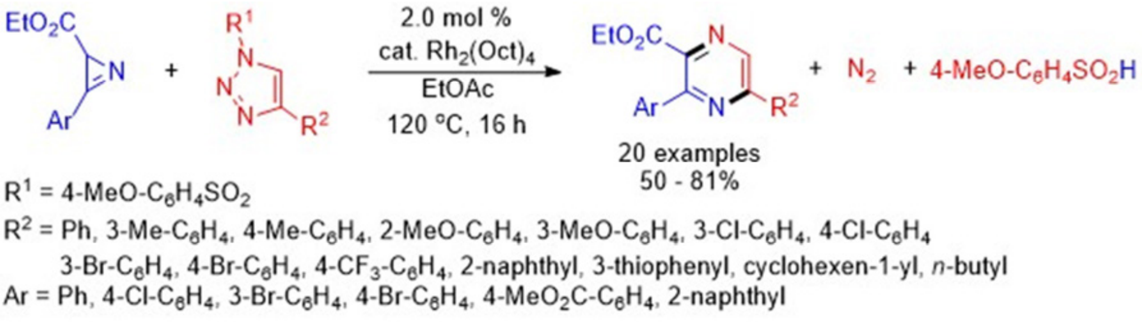
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-320**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Trisubstituted Pyrazines from Rh-Catalyzed Reaction of 2*H*-Azirines with *N*-Sulfonyl-1,2,3-triazoles

김종혜 백용현 이필호*

강원대학교 화학과

Development of a new synthetic method for azaheterocyclic compounds is highly significant in the investigation for new medicines, active pharmaceutical ingredients (API), and fine chemicals. In particular, pyrazine is one of the most representative privileged azaheterocyclic scaffolds, which show cytostatic, antifungal, and antitumor properties and are broadly present in flavorings and alarm pheromones. Accordingly, access to pyrazines from easily available starting materials is highly required. we report herein an efficient synthetic route to a wide range of trisubstituted pyrazines is developed from Rh-catalyzed reaction of 2*H*-azirines with *N*-sulfonyl-1,2,3-triazoles through the elimination of nitrogen molecule and arylsulfinic acid. The present reaction proceeds through formation of *in situ* generated dihydropyrazines.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



R^1 = 4-MeO-$C_6H_4SO_2$
R^2 = Ph, 3-Me-C_6H_4, 4-Me-C_6H_4, 2-MeO-C_6H_4, 3-MeO-C_6H_4, 3-Cl-C_6H_4, 4-Cl-C_6H_4
3-Br-C_6H_4, 4-Br-C_6H_4, 4-CF_3-C_6H_4, 2-naphthyl, 3-thiophenyl, cyclohexen-1-yl, *n*-butyl
Ar = Ph, 4-Cl-C_6H_4, 3-Br-C_6H_4, 4-Br-C_6H_4, 4-MeO_2C-C_6H_4, 2-naphthyl

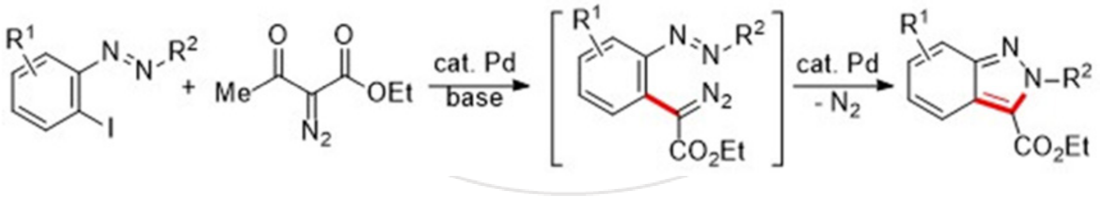
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-321**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Pd-Catalyzed Deacylative Cross-Coupling Reaction and Denitrogenative Cyclization for the Synthesis of 2*H*-Indazoles

윤현식 김지은 이필호*

강원대학교 화학과

A synthetic method to prepare a wide range of 2*H*-indazoles was developed *via* a tandem Pd-catalyzed deacylative cross-coupling reaction of 2-iodoazoarenes and 2-iodoaryltriazenes with acyldiazoacetates and denitroge-native cyclization reaction of *in situ* generated diazoacetates having azoaryl and triazenyl aryl moieties in one-pot. Additionally, azoaryl-substituted diazoacetates underwent Pd-catalyzed denitrogenative cyclization to produce 2*H*-indazoles. The present reaction is a good example in which a Pd(0)-catalyst is involved in two catalytic cycles in one-pot.



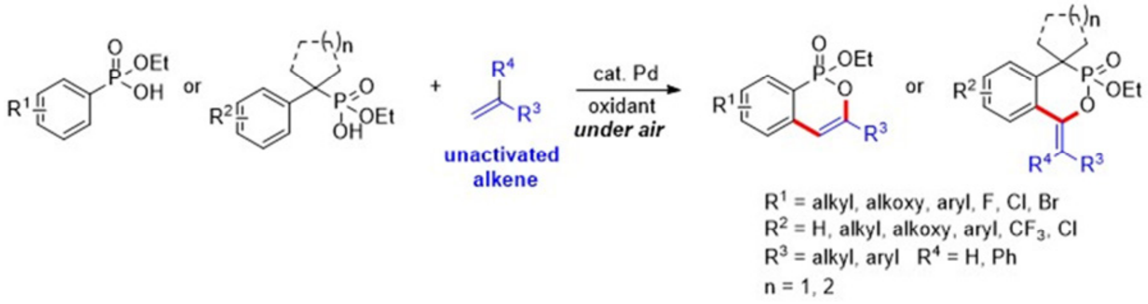
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-322**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Pd-Catalyzed Phosphaannulation for the Synthesis of 3-Substituted Phosphaisocoumarins

윤현식 손정유 이필호*

강원대학교 화학과

An efficient phosphaannulation *via* Pd(II)-catalyzed C–H activation/oxidative cyclization by 6-*endo* mode is reported for the synthesis of 3-substituted phosphaisocoumarins from the reaction of aryl phosphonic acids with unactivated alkenes under aerobic conditions. Also, *α,α*-disubstituted benzyl phosphonic acids were phosphaannulated with unactivated alkenes, producing phosphaisochromanones having (*Z*)-alkylidenyl groups *via* *anti*-phosphoryoxypal-ladation by 6-exo mode.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-323**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dynamic Morphological Transformation for Stimuli Responsive Self-Assembled Peptide Architectures

ZHANGLIANJIN 이희승*

KAIST 화학과

The stimuli responsive self-assemblies have been attracted much interest recently because of their ability to modulate self-assembled morphologies, functions and properties.[1,2] Our group has proved that unnatural β-peptide also can form highly ordered nanostructures and well-defined supra-molecular structures through multiple non-covalent interactions.[3] In this study, we designed and synthesized new peptide with incorporating azobenzene moiety at N-terminus of the β-peptide to create external stimuli responsive self-assembly. Self-assembled microstructures of this peptide presented photo-induced morphological transformation and fluorescence enhancement behavior in water. Furthermore, significant morphological changes with size decrease and phase transition from amorphous to crystalline were observed when heating the self-assembled peptide. This precise control of the self-assembly of stimuli-responsive peptide in molecular level is a challenging goal, which we will succeed in controlling and understanding its important mechanism for fabricating novel functional materials in biomedical applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-324**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of a new privileged substructure-based diversity-oriented synthesis (pDOS) pathway for unprecedented pyrimidine-embedded polyheterocycles

최유나 김희준 박승범*

서울대학교 화학부

For the discovery of novel bioactive chemical entities with new modes of action in the field of drug discovery and chemical biology, the collection of drug-like small molecules with high skeletal diversity plays a pivotal role in the discovery of promising small-molecule ligands using both a conventional target-based approach and a phenotype-based approach. In order to maximize the molecular diversity in such a collection, the biomedical research community has applied diversity-oriented synthesis (DOS) as the major strategy. Along with this endeavor, a privileged substructure-based DOS (pDOS) strategy has emerged for the generation of the novel collection of drug-like small molecules exhibiting high efficiency and improved biological relevance. For maximizing the coverage of chemical space employing pDOS strategy, we focused on the diversification of conformationally restricted polyheterocycles in a three-dimensional (3-D) space.In this regard, we have developed a new pDOS pathway with pyrimidine as a privileged substructure. We pursued the fabrication of unique and unprecedented pyrimidine-embedded polyheterocycles via systematic ring size control. The obtained pDOS library from this strategy ensures high potential for molecular interactions with biopolymers in a selective and specific manner.

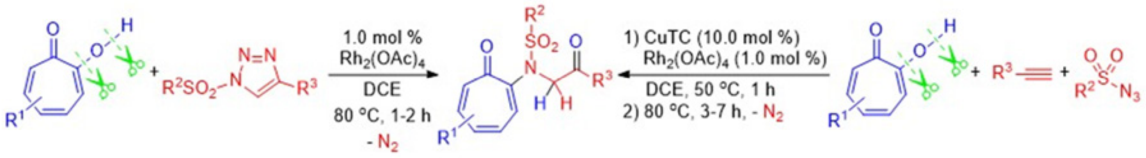
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-325**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of 2-Aminotropones from *N*-Sulfonyl-1,2,3-triazoles and Tropolones

서보람 김야곱 이필호*

강원대학교 화학과

Tropones make up a significant class of seven-membered non-benzenoid aromatic compounds that can be subjected to higher order cycloaddition reactions to provide a large number of biologically active compounds and natural products. Aminotroponimines derived from tropolone having a 2-hydroxy group are also a typical group of ligands. In this regard, introduction of new functional groups onto tropone and transformation of previously present functional groups in the troponoid family are desirable. Although there are several methodologies for the preparation of functionalized tropones in the literature, the development of new and convenient methods to prepare them is imperative.For this reason, we have developed the Rh-catalyzed reaction of tropolones with *N*-tosyl-1,2,3-triazoles for the synthesis of the 2-functionalized aminotropones via tandem Rh-catalyzed O−H insertion, intramolecular 1,8-addition, and rearrangement in one pot. Sequential Cu-catalyzed [3 + 2] cycloaddition, Rh-catalyzed O−H insertion, intramolecular 1,8-addition, and rearrangement starting from 1-alkynes, *N*-sulfonyl azides, and tropolones is also demonstrated for the synthesis of the 2-functionalized aminotropones in one pot. These results suggest that sequential functionalization of O−H and C(sp^2)−O bonds smoothly take place in C(sp^2)−O−H bonds at the 2-position of tropolone.



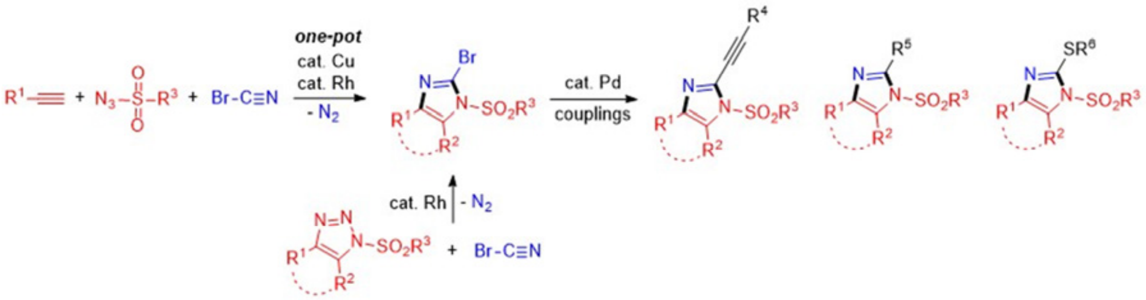
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-326**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rh-Catalyzed Cyclization of *N*-Sulfonyl-1,2,3-triazoles with Bromocyanide for the Synthesis of 2-Bromoimidazole Derivatives

한기욱 손정유 이필호*

강원대학교 화학과

Imidazoles are a significant scaffold of azaheterocyclic compounds, which are extensively used in biologically active compounds, in ionic liquids, and as precursors of stable carbene ligands. Consequently, development of synthetic routes of highly functionalized imidazoles from easily accessible starting materials has been a continuing challenge in modern organic synthesis. We developed a synthetic method for 2-bromoimidazoles from Rh-catalyzed cyclization of *N*-sulfonyl-1,2,3-triazoles with bromocyanides. Cu-catalyzed [3 + 2] cycloiddit-ion followed by Rh-catalyzed cyclization starting from alkynes, *N*-sulfonylazides, and bromocyanides is also demonstrated for *de novo* synthesis of 2-bromoimidazoles in one pot. Moreover, this work was successfully employed to introduce diverse functional groups to the 2-position of imidazoles *via* cross-coupling reaction.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



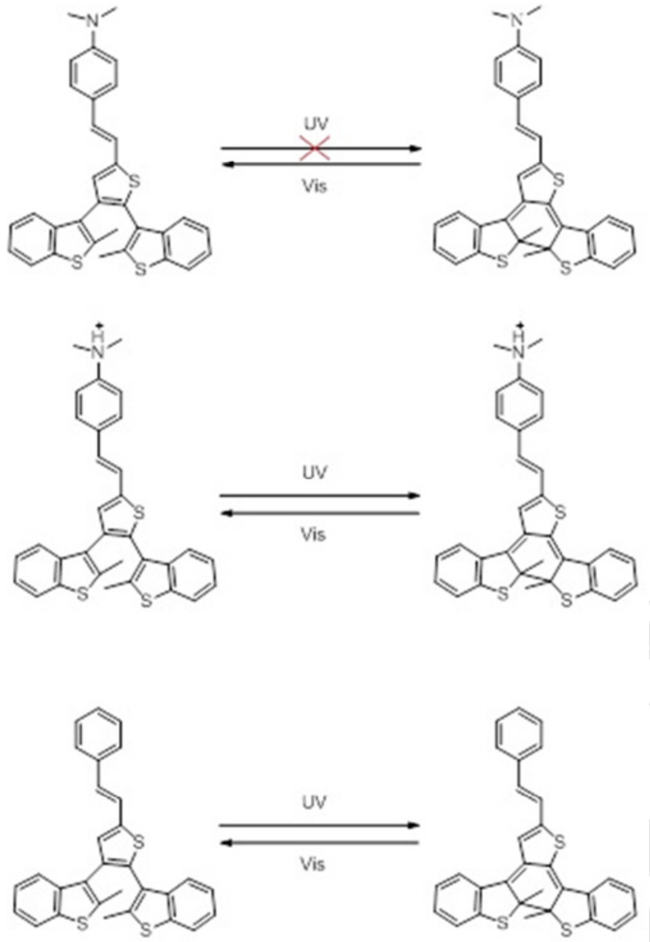
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-327**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Acid catalyzed photoswitching of diarylethenes

홍승주 윤호준 안광현[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

External trigger using light could provide a valuable mean to switch between two different states. There is a need for new and simple protocols to regulate cyclization and cycloreversion of photochromic diarylethenes, which are the most promising materials for the construction of photoswitchable systems because of their excellent thermal stability and outstanding fatigue resistance. Herein, we will show the acid catalyzed cyclization of open form (E)-4-(2-(4,5-bis(2-methylbenzo[b]thiophen-3-yl)thiophen-2-yl) vinyl)-N,N-dimethylaniline to close form under UV light. Without acid, the open form couldn`t transform to close form. In the presence of acid, upon irradiation with UV light, a new band corresponding to the ring closed form at around 560nm was appeared.


UV
Vis
UV
Vis
UV
Vis

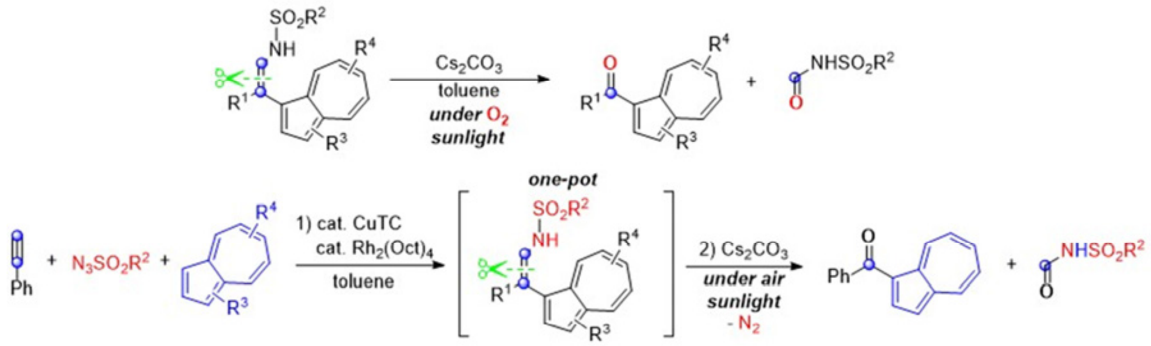
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-328**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Azulen-1-yl Ketones through Oxidative Cleavage of C-C Multiple Bonds

맹찬영 백용현 이필호*

강원대학교 화학과

Azulenes, which are nonbenzenoid aromatic hydrocarbons and nonalternant isomers of naphthalene, are an important class of compounds because of their biological activities and physicochemical properties. Hence, the establishment of a new approach to prepare azulene and its derivatives from easily accessible starting materials is highly desirable. In this regard, the introduction of new functional groups to the azulene ring and the transformation of previously present functional groups are required. The selective introduction of an acyl group to the azulene ring is particularly desirable because of such groups electronic and electrochemical properties.In this context, our group had developed a synthetic method to prepare azulen-1-yl ketones *via* an oxidative cleavage of the C−C double bond in *N*-sulfonyl enamides by the reaction of readily obtainable *N*-sulfonyl enamides with Cs_2CO_3 under air and natural sunlight and in the absence of a photosensitizer. An oxidative cleavage of C−C triple bonds was also demonstrated for the synthesis of azulen-1-yl ketone *via* the tandem Cu-catalyzed [3 + 2] cycloaddition, Rh-catalyzed arylation, photooxygenation, and ring-opening reaction in one pot under air and natural sunlight. Notably, the present method offers a wide range of azulen-1-yl ketones that are difficult to prepare using previously developed tools.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



- ***C-C multiple bond cleavage***
- ***Readily obtainable enamides***
- ***Photosensitizer free***
- ***Under air and natural sunlight***
- ***Easy reaction conditions***

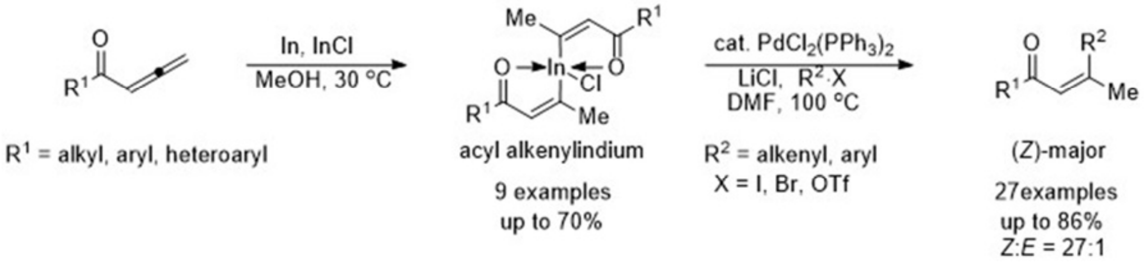
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-329**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of (*Z*)-*α,β*-Unsaturated Ketones through Pd-Catalyzed Cross-Coupling from Acyl Alkenylindium Reagents

맹찬영 전봉근 이필호*

강원대학교 화학과

A synthetic method of acyl alkenylindium reagents was developed from the hydroindation reaction of allenyl ketones with indium and indium chloride in methanol under mild conditions. Their synthetic applications were demonstrated from Pd-catalyzed cross-coupling reactions with aryl bromides and iodides and alkenyl and aryl triflates for the synthesis of (*Z*)-*α,β*-unsaturated ketones.



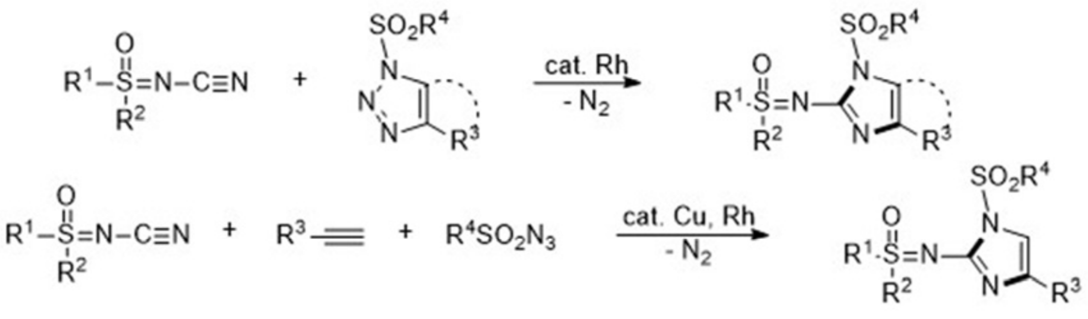
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-330**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rh-Catalyzed *N*-Imidazolylation of Sulfoximines

김상혁 김지은 이필호*

강원대학교 화학과

Sulfoximines are significant privileged scaffolds, which are extensively found in bioactive compounds, chiral auxiliaries, and ligands in asymmetric synthesis. In consequence, the development of efficient synthetic approaches for sulfoximines and their functionalizations have been continuously required. In particular, *N*-(hetero)aryl sulfoximines are attractive due to the fact that a multitude of their derivatives exhibited anticancer activity or proved useful as agrochemicals.Recently, a synthetic method using *N*-sulfonyl-1,2,3-triazoles as precursors of α-imino Rh carbenoid has been widely studied. Especially, Fokin and Lee described that Rh-catalyzed reaction of 1,2,3-triazoles with nitriles and bromocyanides afforded imidazoles and 2-bromoimidazoles, respectively. In our continuing studies related to the synthesis of nitrogen heterocyclic compounds using *N*-sulfonyl-1,2,3-triazoles, we envisioned that if *N*-cyano sulfoximines would be used as nucleophile in reacting with *N*-sulfonyl-1,2,3-triazoles, *N*-imidazolyl sulfoximines would be obtained *via* denitrogenative [3 + 2] cycloaddition. Herein, we demonstrate Rh-catalyzed *N*-imidazolylation of *N*-sulfonyl-1,2,3-triazoles with a variety of *N*-cyano sulfoximines for the synthesis of *N*-imidazolyl sulfoximines *via* elimination of molecular nitrogen. Moreover, Cu-catalyzed [3 + 2] cycloaddition followed by Rh-catalyzed *N*-imidazolylation from 1-alkynes, *N*-sulfonyl azides, and *N*-cyano sulfoximines is developed for the synthesis of *N*-imidazolyl sulfoximines in one-pot.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)


cat. Rh
- N2
cat. Cu, Rh
- N2
R1
R2
R3
R4
SO2R4
R4SO2N3

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-331**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Stable analog of phosphoaspartate (pAsp)

박지효 권기빈[1] 기정민[2,*]

UNIST 나노생명화학공학부 [1]UNIST 에너지및화학공학부 [2]UNIST 화학과

Bacteria and plant cells have two-component regulatory systems (TCS), which serves as the key stimulus-response mechanisms to respond to changes in environmental conditions. A TCS typically consists of a membrane-bound histidine kinase (HK) that senses a specific environmental stimulus and the corresponding response regulator (RR) which has a conserved aspartate residue for the mediation of the cellular responses. The HK undergoes autophosphorylation to form a phosphohistidine (pHis) upon sensing the signal and subsequently phosphorylates the aspartate residue of RR to form an phosphoaspartate (pAsp). This phosphorylated RR induces the target-gene expression/suppression. For the better understand of TCS, the two questions need to be answered; “Among many kinds of HKs and RRs, what signal activates what HKs and then what RRs are activated?” and “What is the clear target of those activated RRs?” Accordingly, the detection and quantification of pAsp levels in proteins is of crucial significance in TCS research, and pAsp-specific antibodies will be invaluable tools. Unfortunately, all the previous efforts to obtain such antibodies have failed due to the chemical instability of pAsp and resultant decomposition of pAsp-containig immunogens in vivo. To address this, we developed stable pAsp analogs to use as the haptens to generate pAsp-specific antibodies. Here we report the design, synthesis, and the utilization of the analog.

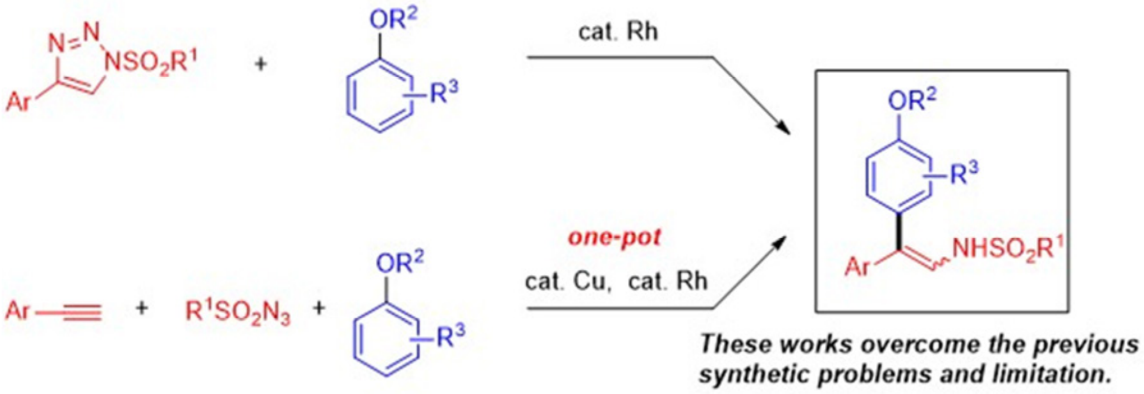
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-332**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Cu-Catalyzed Cycloaddition and Rh-Catalyzed Alkoxyarylation for the Synthesis of 2-Alkoxyaryl-2-aryl Enamines in One-Pot

김야곱 손정유 이필호*

강원대학교 화학과

An efficient synthetic method to a myriad of 2,2-diaryl enamines is developed from Rh-catalyzed arylation of *N*-sulfonyl-4-aryl-1,2,3-triazoles with aryl ethers *via* the elimination of nitrogen molecule. Cu-catalyzed cycloaddition followed by Rh-catalyzed arylation starting from alkynes, *N*-sulfonyl azides, and aryl ethers is also demonstrated for synthesis of 2,2-diaryl enamines in one-pot.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



These works overcome the previous synthetic problems and limitation.

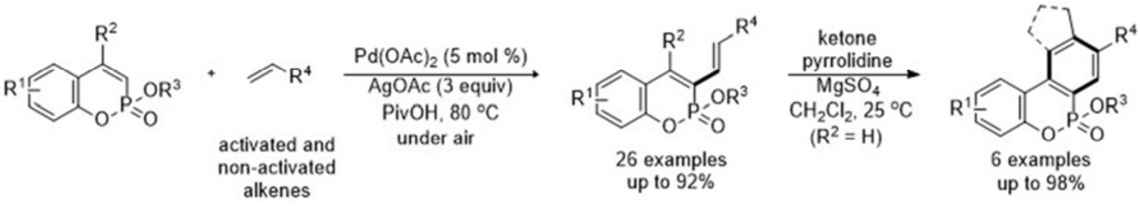
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-333**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Benzophosphacoumarine Derivatives *via* Pd-Catalyzed C-H Alkenylation

김야곱 이진섭 이필호*

강원대학교 화학과

For several decades, organophosphorus compounds have received attention due to applications in diverse fields such as coordination and materials chemistry, homogeneous catalysis, pharmaceuticals, agrochemicals, additives for polymers, and flame retardants. We were attracted to developing a streamlined method for the synthesis of a myriad of phosphacoumarins and benzophosphacoumarins with the aim of making useful chemical libraries and probes. In addition, the importance of cross-dehydrogenative coupling reactions on Pd-catalyzed direct C–H alkenylation of heteroarenes has been rapidly increased. Herein, we have developed an oxidative alkenylation from the reaction of phosphacoumarins with a wide range of activated as well as non-activated alkenes *via* aerobic oxidative Heck reactions. Moreover, 3-alkenylphosphacoumarins undergo inverse electron demand Diels-Alder reaction with enamines *in situ* generated from ketone and pyrrolidine followed by 1, 2-elimination and a dehydrogenation, affording fluorescent benzophosphacoumarins.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-334**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

9-Fluorenylmethyl (Fm) disulfides: preparation, reactivity, and use as convenient precursors for persulfides

박정민

강릉원주대학교 화학신소재

Hydrogen sulfide (H_2S) is an important biological signaling agent that exerts action on numerous physiological processes through the S-sulfhydration of biological molecules, such as cysteine residues (RSH), forming persulfides (RSSH). We are interested in developing chemical tools to explore generation and reactivity of perulfides. We recently discovered a functional disulfide, FmSSPy-A (Fm = 9-fluorenylmethyl; Py = pyridinyl) that enables both small molecules and protein thiols (R-SH) to effectively convert R-SSFm adducts as persulfide precursors. We will describe this method allowing for a H_2S-free and biomimetic protocol to generate highly reactive persulfides.

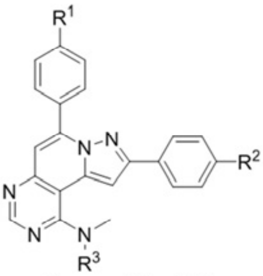
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-335**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A pyrazolo[1,5-a]pyridine-fused pyrimidine based novel fluorophore and its bioapplication to probing lipid droplets

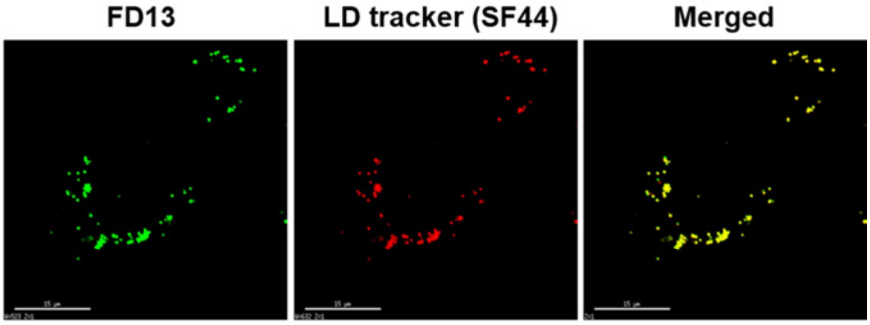
김희준 조아라 하재영[1] 이영준 황윤수 박승범*

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

A new fluorescent core skeleton containing pyrazolo[1,5-a]pyridine-fused pyrimidine, called fluoremidine (FD), was discovered. FD analogues were prepared via a one-pot silver-catalyzed cascade cyclization. An N,N-dimethylamino group at the R1- and R2-positions plays important roles in controlling fluorescence brightness and emission wavelength. An N-acetyl group at the R3 position contributes to red shifting of the emission wavelength. FD shows excellent solvatochromism with turn-on fluorescence in the lipophilic environment, which was utilized to design a fluorescent probe, FD13, for visualizing lipid droplets in living cells.



Fluoremidine (FD)



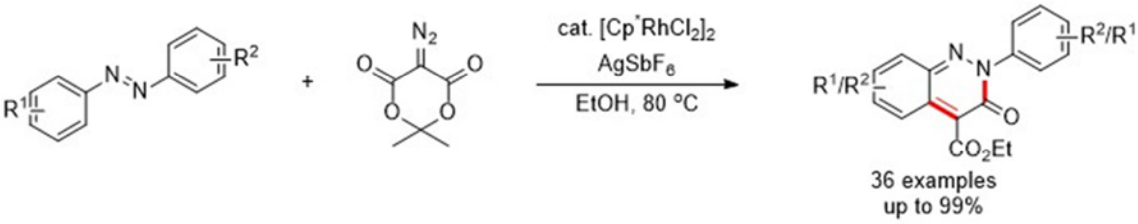
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-336**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Cinnolin-3(2*H*)-ones *via* Rh-Catalyzed Cyclization of Azobenzenes with Diazotized Meldrum's Acid

전다혜 전보미 이필호[*]

강원대학교 화학과

Nitrogen heterocycles are a very significant class of compounds because of their pharmaceutical applications and biological activities. Especially, cinnolin-3(2*H*)-ones are constituents of key privileged azaheterocyclic scaffolds. Thus, the establishment of robust synthetic approaches for affording substituted cinnolin-3(2*H*)-one from easily available compounds has been continuously demanded. Recently, we reported a myriad of C−H activation using phosphoryl group as a directing group and an efficient synthetic method of 2-aryl-2*H*-benzotriazoles from azobenzenes and *N*-sulfonyl azides *via* sequential Rh-catalyzed amidation and oxidation in one pot. In our current program involved with the synthesis of nitrogen heterocycles using azobenzenes, we envisioned that reaction of azobenzenes with diazotized Meldrum's acid would provide a cinnolin-3(2*H*)-one skeleton. Herein, we describe a synthetic method of a wide range of cinnolin-3(2*H*)-one derivatives is developed from the reaction of symmetrical as well as unsymmetrical azobenzenes with diazotized Meldrum's acid *via* Rh-catalyzed C−H alkylation followed by cyclization.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



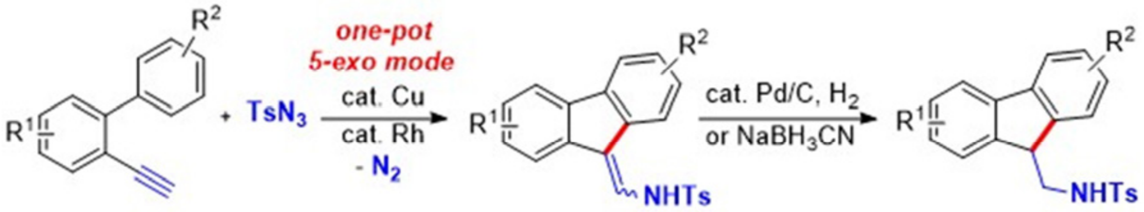
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-337**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rh-Catalyzed Denitrogenative Cyclization of *N*-Sulfonyl-4-biaryl-1,2,3-triazole for the Synthesis of Fluorenes

전다혜 윤현식 이필호*

강원대학교 화학과

Fluorenes have attracted a great deal of attention due to their optical and electronic properties and their function as π-conjugated materials. They have been widely used as significant privileged structure in a myriad of areas such as optical agents, dyes, organic transistors, and light-emitting devices. Hence, an efficient synthesis of fluorene and its derivatives from easily available compounds has been continuously required. Especially, it is very important to prepare selectively unsymmetrically substituted fluorene derivatives and to introduce substituents at the C-9 methylene bridge of the fluorene moiety without use of base.We report an efficient synthetic method of a wide range of unsymmetric fluorenes having enamine moiety at C-9 methylene bridge from *N*-sulfonyl-4-biaryl-1,2,3-triazole derivatives *via* Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode. Rh-catalyzed denitrogenative cyclization followed by catalytic hydrogenation produces the aminomethyl-substituted fluorenes in a one-pot. Moreover, this protocol can be applied the synthesis of fluorenes *via* tandem Cu-catalyzed [3 + 2] cycloaddition and Rh-catalyzed denitrogenative cyclization in a 5-*exo* mode starting from 2-ethynylbiaryls and *N*-sulfonyl azides in a one-pot.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



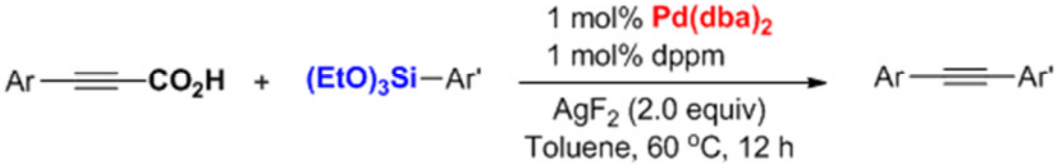
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-338**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Diarylalkynes using Palladium-Catalyzed Decarboxylative Coupling Reaction from Alkynyl Carboxylic Acids and Arylsiloxanes

장지선 손유정 이선우*

전남대학교 화학과

Organosilanes have been used as coupling partners less than other coupling reagents, such as aryl halide and organoborane, even though they are stable, inexpensive, non-toxic, and easily prepared. Also Organosilanes have been employed as coupling partners in palladium-catalyzed cross coupling reactions since Hiyama first reported the coupling of aryl halides and arylsiloxanes in 1988. But The decarboxylative coupling reaction of organosilane is a recondite branch. Very recently, we reported a decarboxylative coupling reaction with organosilane using a nickel catalyst, which provided the diaryl alkyne in moderate to good yields. However this reaction with organosilane using a palladium catalyst is still unknown. So we study this reaction and succeed to develop of palladium catalytic system with arylsiloxane. According to the results of the experiment, This method provided the desired coupled products in moderate to good yields by reacting the alkynyl carboxylic acids and arylsiloxanes with $Pd(dba)_2$ (1.0 mol%), 1,1-bis(diphenylphosphino)methane (1.0 mol%), and AgF_2 (2.0 equiv) at 60 ^{o}C for 6 h. It is milder than the reaction with arylsiloxane using nickel catalyst, because amount of the catalyst is less than amount of nickel catalyst and the reaction temperature of palladium catalytic system is lower than the reaction temperature of nickel catalytic system.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-339**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Glycero-D-Manno-Heptose-7-Phosphate Derivatives

김예림 권용억*

이화여자대학교 화학.나노과학과

Heptoses are common constitutuents of the inner core region of lipopolysacharides (LPS) which are essential components of the outer membrane of Gram-negative bacteria. LPS mediate numerous immunological and pathophysiological responses in bacterial infections. Heptoses have been found in L-glycero-D-manno or D-glycero-D-manno forms depending on the different bacterial strains. Melioidosis is an infectious disease which is caused by Burkholderia pseudomallei, found in water or soil. The heptose biosynthetic pathway of Burkholderia pseudomallei associated in melioidosis includes some heptose-based carbohydrate derivatives catalyzed by several enzymes such as kinases, phosphatases and isomerases. In this presentation, we report the efficient synthesis of several glycero-D-manno-heptose-7-phosphate derivatives which can be possible inhibitors or substrates against kinases in the heptose biosynthetic pathway.

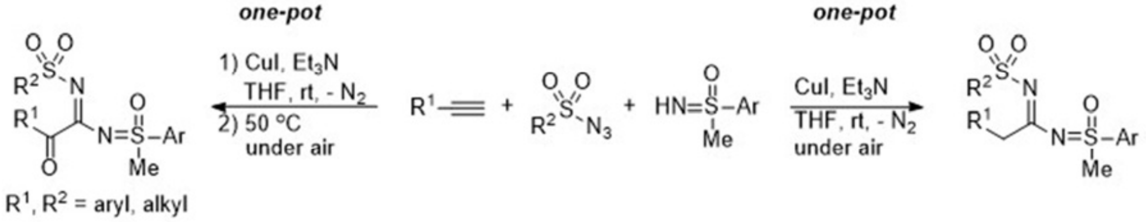
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-340**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Cu-Catalyzed *N*-Imidoylation from Alkynes, *N*-Sulfonyl Azides, and Sulfoximines

전보미 손정유 이필호*

강원대학교 화학과

N-Imidoylation of sulfoximines is developed from a Cu-catalyzed three-component reaction from 1-alkynes, *N*-sulfonyl azides, and sulfoximines in THF at room temperature under air. In addition, *N*-oxoimidoylation of sulfoximines is accessed from a Cu-catalyzed three-component reaction from 1-alkynes, *N*-sulfonyl azides, and sulfoximines in THF at room temperature followed by a Cu-catalyzed oxidative reaction at 50 °C under air, producing *N*-oxoimidoyl sulfoximines. This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



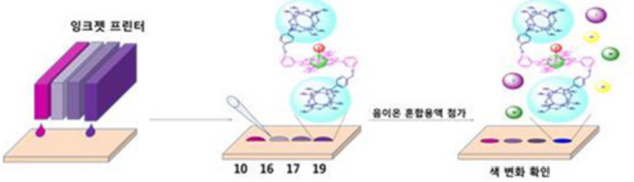
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-341**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Inkjet Print Technique toward the Fabrication of POSS-Porphyrin Sensors

정은희

강릉원주대학교 화학신소재학과

We have succeeded in the fabrication of the series of porphyrin derivatives which incorporating polyhedral oligomeric silsesquioxanes (POSS) units. Studies on their synthesis, characterization of their spectroscopic properties and the cellular uptake properties with Cos-7 cells have been performed. However their applications as chemical sensors or drug delivery carriers were prevented by their poor solubility in most organic solvents. Here we report a method that uses inket printing to make POSS-Porphyrin Sensors. Using the standard commercial inkjet printer, we can print the various POSS-Porphyrin derivatives on the paper strips. This technique will allow us not only to avoid solubility problem but also to provide the new method for the generation of the real shape-selective POSS-Porphyrin Sensors.


잉크젯 프린터
10
16
17
19
음이온 혼합용액 첨가
색 변화 확인

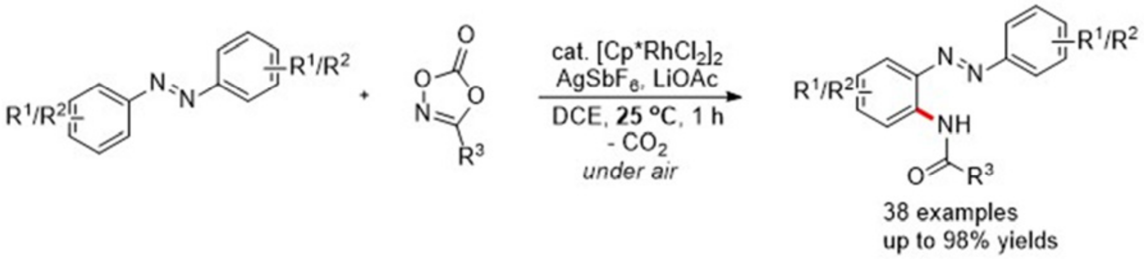
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-342**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Selective Rhodium-Catalyzed C−H Amidation of Azobenzenes with Dioxazolones under Mild Conditions

전보미 손정유 이필호*

강원대학교 화학과

Azobenzenes are a significant class of compounds in many fields, such as organic dyes, food additives, and material science. Thus, development of streamlined synthetic methods for their derivatives is greatly needed. Although the introduction of a wide range of functional groups onto a symmetrical azobenzene ring has been reported, selective introduction of substituents onto unsymmetrical azobenzenes still represents a formidable challenge. In our continuing efforts in C−H activation, we have been interested in the development of direct and selective C−N bond formation using both symmetrical and unsymmetrical azobenzenes under mild conditions. Herein, we present an efficient synthetic method for a wide range of amidated azobenzenes through the selective Rh-catalyzed C−H amidation reaction of symmetrical as well as unsymmetrical azobenzenes with alkyl-, aryl-, and heteroaryl-substituted dioxazolones under mild conditions. In addition, diamidation of azobenzenes and amidation of monoamidated azobenzenes will be presented.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-343**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Stimuli-degradable dendrimers with hexahydro-triazine core for siRNA delivery

조수경 김은비 정대일* 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

RNA interference (RNAi) has immense potential as therapeutic strategy to knockout disease genes. However, in order to successfully translate RNAi into clinic, safe and efficient delivery of small interfering RNA (siRNA) to target tissue must be resolved. Among various delivery vehicles, dendrimers offer interesting properties such as highly defined structure, multivalency, and molecular uniformity, which make them an attractive candidate. Polyamidoamine (PAMAM) and their derivatives are the most widely studied dendrimers. While the biological activities of the dendrimer are governed mostly by the peripheral groups and generation numbers, numerous studies have also suggested that the dendrimer core flexibility also play a significant role. Moreover, despite extremely low polydispersity and molecular homogeneity, dendrimers still pose toxicity issues stemming from large molecular weight and large surface area. Therefore, biodegradable dendrimer, which upon successful delivery, is degraded into harmless small molecules, is greatly desired. In this study, stimuli-responsive hexahydro-triazine dendrimer is synthesized from amino acid, cysteine, with biodegradable branches. Our synthetic strategy allowed the preparation of dendrimer core with high degree of freedom triazine ring in high yields using relatively green and safe chemistry. Incorporating biodegradable linker in the branch is anticipated to decrease the cytotoxicity as well as possible side effects. Different branches including linear polyethylenimine and poly-L-lysine are also grafted for comparison. Cytotoxicity of dendrimers as well as their ability to complex and deliver nucleic acid therapeutics is studied.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-344**

발표분야: 유기화학

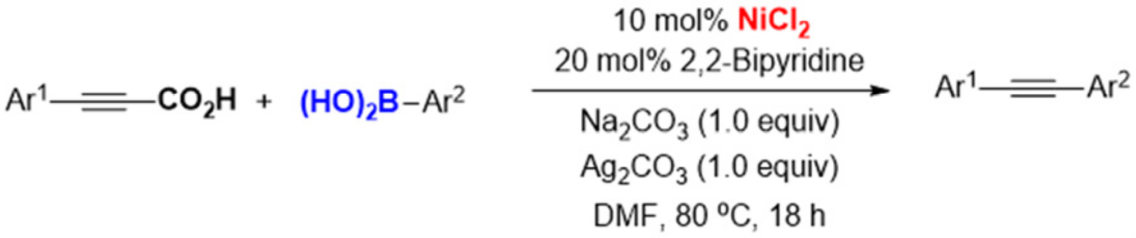
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-pot synthesis of Diaryl Alkynes : Nickel-Catalyzed Oxidative Decarboxylative Coupling Reactions with Alkynyl Carboxylic Acids and Aryl Boronic Acids

이주현 박재림 이선우*

전남대학교 화학과

Decarboxylative coupling reactions were generally employed as major catalysts such as palladium or copper, although a few example of nickel catalysts were reported. For example, we recently described decarboxylative coupling reactions with organosilanes using a nickel catalyst. This success prompted us to develop a nickel-catalyzed decarboxylative coupling using organoboranes. Although the oxidative decarboxylative coupling with aryl boronic acids was reported in the presence of a palladium and copper catalyst, a nickel-based catalytic system has not been developed so far. Therefore, we study a decarboxylative coupling reaction between alkynyl carboxylic acids and organoboranes using a nickel catalyst.Thus we developed Ni catalyzed decarboxylative coupling reaction of alkynyl carboxylic acids with aryl boronic acids. When aryl alkynyl carboxylic acids were reacted with aryl boronic acids in the presence of $NiCl_2$ (10 mol%), 2,2-bipyridine (20 mol%), Na_2CO_3 (1.0 equiv), and Ag_2CO_3 (1.0 equiv) in DMF at 80 °C for 18 h. The corresponding diaryl alkynes products were formed in moderate to good yields.



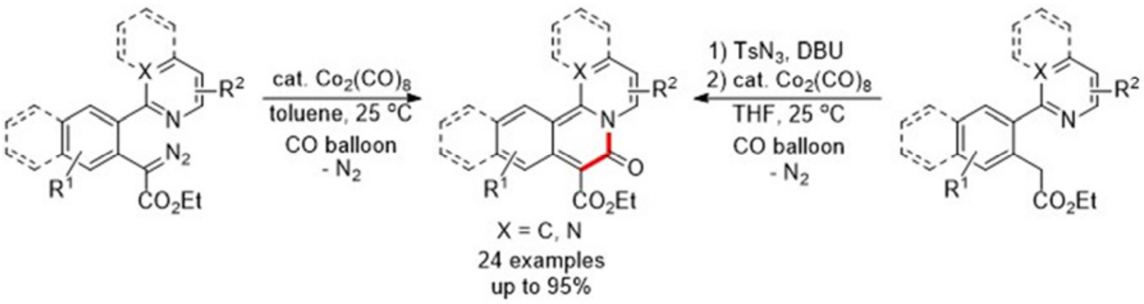
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-345**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Pyridoisoquinolinones *via* Co-Catalyzed Carbonylative Cyclization of Pyridinyl Diazoacetates

<u>백용현</u> 전봉근 이필호*

강원대학교 화학과

Dicobalt octacarbonyl-catalyzed carbonylative cyclization of pyridinyl diazoacetates is developed for the synthesis of pyridoisoquinolinones under mild conditions (room temperature) in a carbon monoxide atmosphere. Moreover, a useful synthetic method for a wide range of pyridoisoquinolinones from pyridinyl aryl acetates has been demonstrated through diazotization using TsN_3 and DBU followed by Co-catalyzed carbonylation and intramolecular cyclization of ketene with a tethering pyridinyl moiety under a carbon monoxide atmosphere in a semi-one-pot procedure. These transformations are attractive due to the use of an inexpensive and commercially available Co catalyst and an easily accessible starting material and the release of harmless N_2 under mild conditions (room temperature).This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



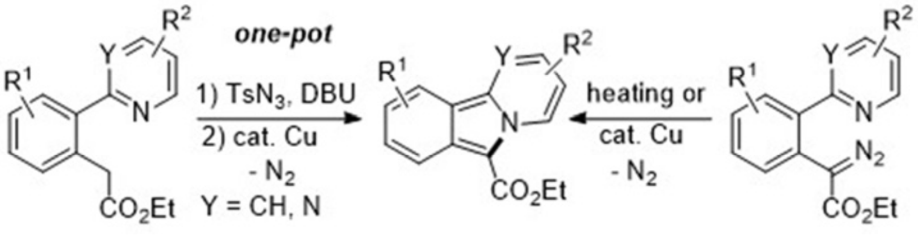
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-346**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Diazotization/Intramolecular Cyclization for the Synthesis of Pyridoisoindole Derivatives

백용현 이진섭 이필호*

강원대학교 화학과

Pyridoisoindoles are key priviledged scaffolds in nitrogen-containing heterocyclic compounds, which are widely found in pharmaceuticals, natural products, fluorescent materials, and dyes. Accordingly, development of synthetic methods for preparing pyridoisoindoles having a variety of functional groups represents a considerable task and a significant challenge. Although these functionalizations of pyridoisoindole derivatives have been reported, a limited number of synthetic methods have been described. Thus, a robust synthesis of pyridoisoindole derivatives has been continuously needed. Especially, it is very significant to introduce a wide range of functional groups onto pyridoisoindoles and to prepare 6-ethoxycarbonyl pyridoisoindoles. Moreover, preparation of pyridoisoindole derivatives having other nitrogen heterocycles besides pyridine provides a synthetic challenge.Herein, we have developed a robust synthetic method for a wide range of pyridoisoindoles from pyridinylarylacetates in one-pot through diazotization using TsN_3 and DBU followed by intramolecular cyclization *via* elimination of nitrogen molecule under $Cu(OTf)_2$-catalyzed conditions. Also, the intramolecular cyclization took place efficiently with diazo substrates to furnish pyridoisoindoles in good to excellent yields under metal-free conditions or $Cu(OTf)_2$-catalyzed conditions at room temperature.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (NRF-2015H1C1A1035955)



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-347**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Salicylimine-based Schiff base probe for cascade sensing of Al^{3+} and $^{F-}$ ions

박상아 조효이 서한솔[1] 김홍석[*]

경북대학교 응용화학과 [1]경북대학교 응용화학공학부 응용화학전공

A fluorescent probe comprised of a simple salicylimine-based Schiff base (1) has been developed for sensing Al^{3+} with nano-molar sensitivity in aqueous media. This *turn-on* probe (1) with Al^{3+} was applied to study anions sensing in ethanol led to *turn–off* sensitivity of 1-Al^{3+} complex for F^-. In contrast to ethanol, in methanol media 1-Al^{3+} complex showed *turn-on* response with F^-. Sensing ability of probe and its Al^{3+} complex towards anions will be demonstrated using UV-vis, fluorescence and ^1H NMR studies.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-348**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Trithiane-based hydrogen sulfide donors and their biological evaluations

정의균 박정민[1,*]

강릉원주대학교 화학과 [1]강릉원주대학교 화학신소재

Hydrogen sulfide (H_2S) is known for its characteristic smell of egg rotten. It has been recently recognized as the third physiological gaseous mediator along with CO and NO involved in several physiological processes including hypertension, inflammation, pain perception, anticancer effects, etc. This perspective fuels development of a wide range of H_2S donors in order to understand the physiological roles of H_2S and their therapeutic applications. Our group is interested in developing controllable H_2S donor. We recently synthesized several trithiane-based H_2S donors and performed their biological evaluations. We will report some detailed results of these H_2S donors including syntheses, H_2S concentration measurement, and biological effects.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-349**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Simple one-pot synthesis of bimetallic Pd–Pt–Fe_3O_4 nanoflakes and their performance as magnetically recyclable catalysts nitroarene reduction

변상문 김병문*

서울대학교 화학부

Recently, we have reported several useful catalytic reactions based upon Pd–Fe_3O_4 heterodimeric nanocrystals as novel magnetically recyclable catalysts. Successful applications of the nanocrystals toward various organic reactions such as Heck, Suzuki, and Sonogashira coupling reactions, direct C–H activation reaction, and Wacker oxidation have been reported. In transition metal catlaysis, combination of two metal catalysts sometimes leads to a new synergistic catalyst system. Now, we report the synthesis of bimetallic nanoflake-shaped Pd–Pt–Fe_3O_4 nanoparticles (NP's) and their application to the reduction of nitro- compounds. Using simple hydrothermal procedure, we decorated nano sized crystals of platinum and palladium on the Fe_3O_4 NPs' surface. The nanoflake-shaped Pd-Pt–Fe_3O_4 NPs were very efficient for the one-pot cascade catalysis of dehydrogenation of ammonia borane and reduction of nitro compounds to anilines in methanol at room temperature. Development of efficient methods for the reduction of nitro compounds becomes one of the important synthetic methods in relation with the advent of various medicinal and display materials. The reactions using the Pd–Pt–Fe_3O_4 catalyst proceeded faster than those using either Pd–Fe_3O_4, Pt–Fe_3O_4 or the combination of both Pd–Fe_3O_4 and Pt–Fe_3O_4 catalysts, confirming a unique "synergistic effect" of the bimetallic nano-catalyst system. The catalyst could be recycled through the use of an external magnet in a very straightforward manner and was reusable for over 250 times without loss of its catalytic activity. Thus, this new catalyst could offer a very sustainable, useful and environment-friendly tool for potential industrial applications in the reduction of nitro compounds.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-350**

발표분야: 유기화학

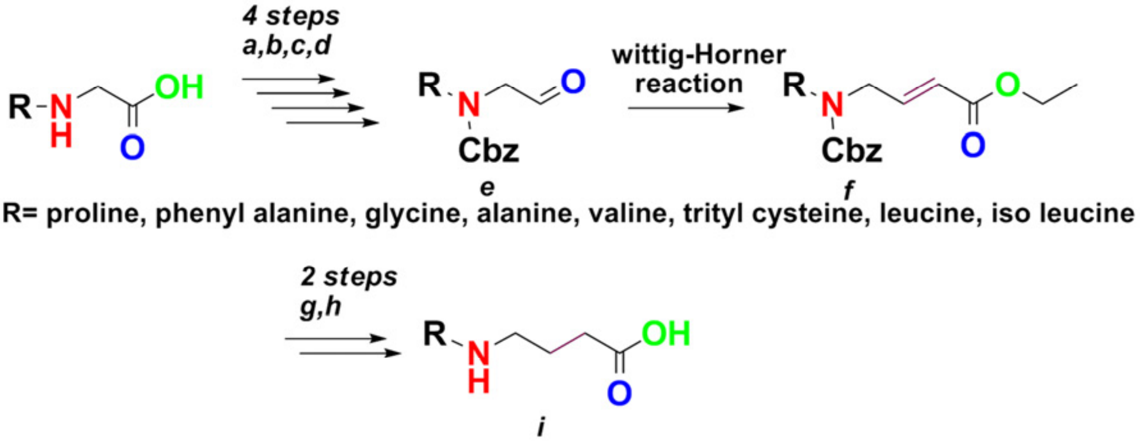
발표종류: 포스터, 발표일시: 금 11:00~12:30

Design & Synthesis of Amino acids (α-amino acid to γ- amino acid) transformation

<u>VAIDYARAGHAVENDERRAO</u> 신동수* chirumarrysridhar PATILKALPESHTUMADU

창원대학교 화학과

Chiral amino acids were commercially available and biologically widely useful compounds. With those we synthesized from α- to γ-amino acids with benzyl carbonochloridate is initial step for amine protection then esterification followed by methyl iodide to convert benzyl protected • • α-amino acid to ester. Ester reacts with sodium borohydride will give alcohol followed by reduction then oxidation of alcohol by using swern oxidation gives aldehyde is the beginning step to get our γ-amino acid. Then the key step for installing α-to γ-carbon enantiomerically pure by using Wittig-Horner reaction with triethylphosphanoacetate gives (E)-benzyl 2-(3-ethoxy-3-oxoprop-1-en-1-yl)pyrrolidine-1-carboxylate (i) if proline is our starting material then a simple hydrolysis, hydrogenation gives chiral γ-mino acid which may biologically useful alternatives to GABA (• • γ-aminobutyric acid)



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-351**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Covalent Conjugation of Small-Molecule Adjuvants to Nanoparticles Induces Robust Cytotoxic T Cell Responses via DC Activation

김우겸 홍성유[1,*]

UNIST 화학공학과 [1]UNIST 나노생명화학공학부

Specific recognitions of pathogen associated molecular patterns by Toll-like receptors (TLRs) initiate dendritic cell (DC) activation, which is critical for coordinating innate and adaptive immune responses. Imidazoquinolines as small-molecule TLR7 agonists often suffer from prompt dissemination and short half-life in the bloodstream, preventing their localization to the corresponding receptors and effective DC activation. We postulated that covalent incorporation of imidazoquinoline moieties onto the surface of biocompatible nanoparticles (～30 nm size) would enhance their chemical stability, cellular uptake efficiency, and adjuvanticity. The fully synthetic adjuvant-nanocomplexes led to successful DC activation at lower nanomolar doses compared with free small-molecule agonists. Once a model antigen such as ovalbumin was used for immunization, we found that the nanocomplexes promoted an unusually strong cytotoxic T lymphocyte response, revealing their unique immunostimulatory capacity benefiting from multivalency and efficient transport to endosomal TLR7.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-352**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Comparative Studies emphasizing the Microwave-assisted *Meta*-selective direct arylation using Homogeneous and Heterogeneous Cu catalysts

양현지 홍성유*

UNIST 나노생명화학공학부

There have been an immense progress in strategies for achieving *meta*-selectivity in the recent years. However, it still remains a serious task to develop a time-efficient and an atom-economical methodology. Herein, we report for the first time, a microwave-enhanced copper-catalyzed *meta*-selective C–H functionalization of pivanilides using symmetrical or unsymmetrical diaryl-iodine(Ⅲ) reagents. This approach apart from being a simple protocol for remote C-H functionalization, has an added advantage of causing extreme reduction in the reaction time. Additionally, we have envisaged, a reaction comparison between homogeneous and heterogeneous Cu catalysts. A wide range of substrate and salt scope has also been explored as well, which included electron-rich, electron-deficient, sterically hindered and heterocyclic motifs.

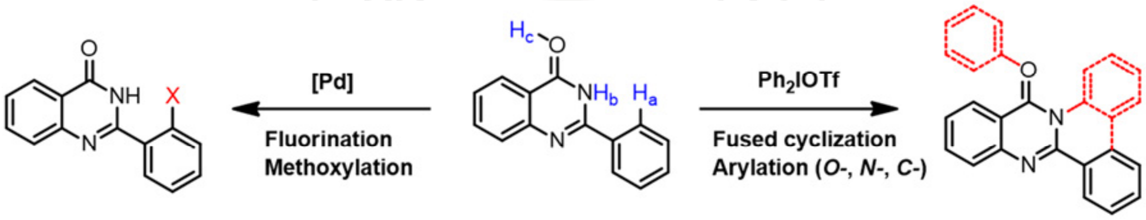
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-353**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Divergent Functionalization of 2-Phenyl-4(3H)-Quinazolinone Derivatives : A Stepping-Stone to Late-Stage Functionalization

이재빈 홍성유[1,*]

UNIST 화학공학부 [1]UNIST 나노생명화학공학부

Selective functionalization in the presence of competing active sites have been a prominent area of organic synthesis. Especially, achieving divergent functionalization of pharmaceutically significant late-stage compounds emerged as one of the most interesting issues to chemists due to its versatility and valuableness. Without installation of external directing groups, our group pioneered late-stage diversification from simple 2-Phenyl-4(3H)-quinazolinone derivatives as a representative of pharmaceutically significant late-stage compounds. Herein, we describe chemo-selective arylation (O-, N- and C-), fused cyclization and divergent C-H functionalization (methoxylation and fluorination) to encourage advance in the area of drug discoveries and late-stage functionalization.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-354**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

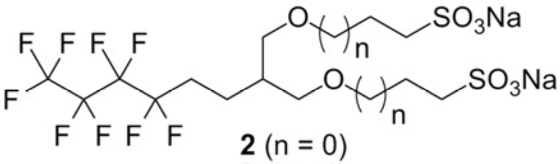
Design, synthesis and property studies of semifluorinated mono, bis, tris and cyclic sulfonated surfactants

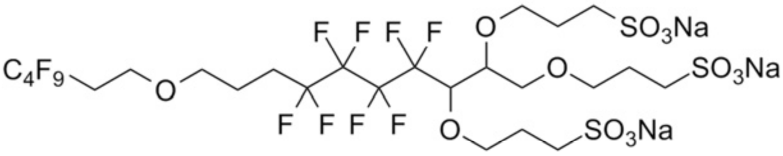
<u>VAIDYARAGHAVENDERRAO</u> 신동수* **chirumarrysridhar PATILKALPESHTUMADU**

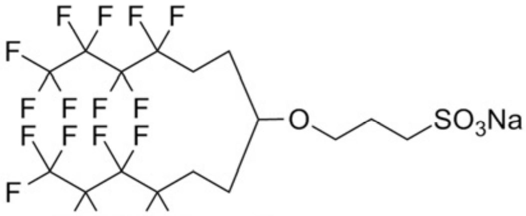
창원대학교 화학과

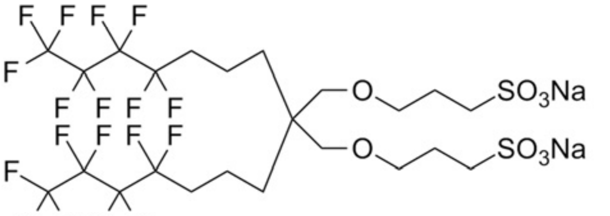
Linear C4-C4 ether linked perfluorobutyl substituted trisodium sulfonates derivatives are designed, synthesized and characterized as alternative substances to perfluoroctanesulfonic acid (PFOS, 1), which have been used as surfactant in various industrial and consumer products. The trisodium sulfonate was synthesized from commercially available octafluoro-1,4-diiodo butane as starting material in 9 steps by using radical addition, Upjohn dihydroxylation and nucleophilic substitution reactions. After successful synthesis of semifluorinated unbranched ether linked trisodium sulfonate we studied surface tension behavior and critical micelle concentration values, along with this material we synthesized di-branched C4-C4 perfluorobutyl alkyl mono sodium sulfonate, bis sodium sulfonate values were noted for comparing activity.

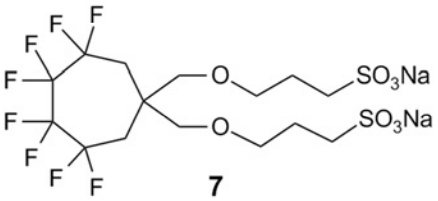

1


2 (n = 0)
3 (n = 1)


4


5


6


7

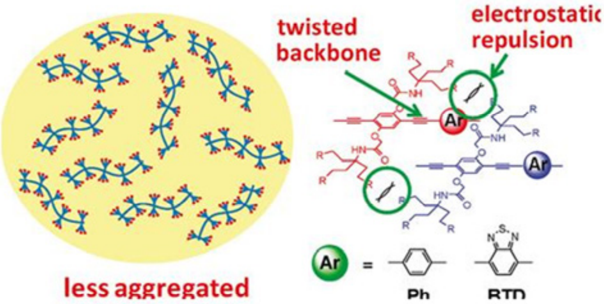
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-355**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Wate-Soluble Conjugated Polyelectrolytes with Branched Polyionic Side Chains

정수진 이성호*

대구대학교 화학응용화학과

A new series of conjugated polyelectrolytes (CPE) consisting of an arylene-ethynylene backbone featuring phenyl (Ph),2,1,3-benzothiadiazole (BTD),or 4,7-bis(2′-thienyl)-2,1,3-benzothiadiazole (TBT) units have been synthesized and characterized. On each polymer repeat unit the CPEs contain two branched ionic side groups each featuring a “triad” of carboxylate (R-$CO_2^-Na^+$) or ammonium(R-$NH_3^+Cl^-$)units, giving the of the series of CPEs were investigated in CH_3OH and H_2O solution by absorption, steady-state fluorescence, and fluorescence lifetime spectroscopy. The different arylene units in the backbone lead to the variation of the HOMO-LUMO gap across the series. The branched, polyionic side chains suppress aggregation of the polymer chains, even in aqueous solution, leading to higher fluorescence quantum yields relative to similar CPEs with linear side chains. UV-vis absorption spectra show that CPEs with anionic branched side chains (R-$^bCO_2^-Na$) aggregate at low pH, while retaining the photophysical properties of their organic-soluble precursors at high pH. CPEs having branched cationic side chains(R-$^bNH_3^+Cl^-$)exhibit the opposite response to pH change.


twisted backbone
electrostatic repulsion
Ar
R
NH
HN
O
Ar =
Ph
BTD
less aggregated

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-356**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of heteroaromatic compounds with Tropane and Pyranosyl rings

배송미 이언진 한정태[1] 정대일[*]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Tropane alkaloids occur naturally in many members of the plant family Solanaceae. In particular, our group is interested in 8-azabicyclo[3.2.1]octan-3-ones because of their pharmaceutical significance and the subsequent modification with pyranosyl groups. Pyranose derivatives are reported to possess antiviral activity with low side effects. Combining this unique characteristic of the pyranose scaffold with 8-azabicyclo[3.2.1]octan-3-ones is anticipated to enhance the physiological activity, the structural specificity, and the biological activity while reducing undesired side effects. Generally, 8-azabicyclo[3.2.1]octan-3-ones can be obtained by the reaction of amines, 2,5-dimethoxy-tetrahydrofuran, and 1,3-acetonedicarboxylic acid. Pyranosyl derivatives can be obtained by the treatment of amines and pyranoses (glucose, mannose, or galactose) in methanol. Catalysts were carefully selected according to the diamino groups. After stirring at room temperature for 12 h, resulting products having a pyranosyl group were recrystallized over 24 h below 4˚C. Synthetic approach reported in this study to prepare heteroaromtic or aliphatic compounds with tropane and pyranosyl groups is efficient way to obtain novel peptidomimetics towards systematic drug discovery.

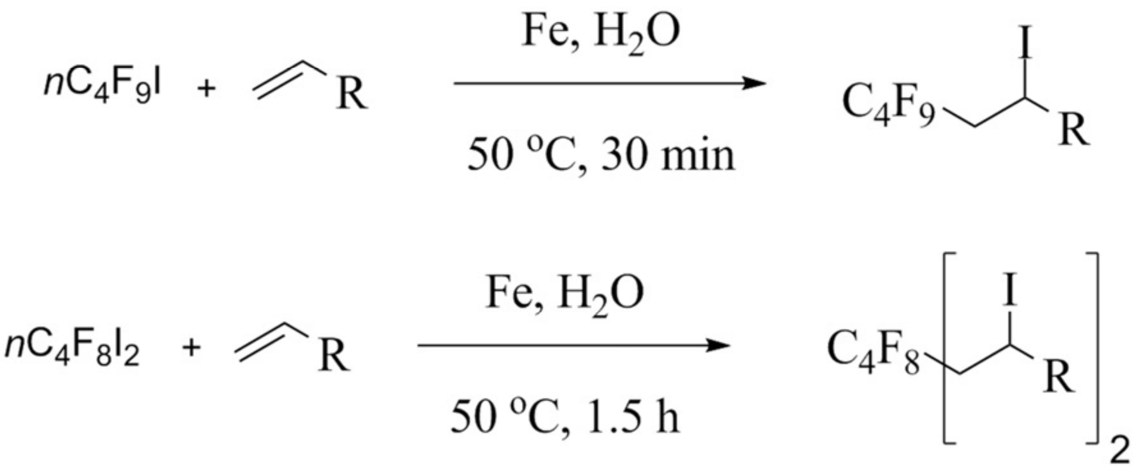
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-357**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Iron-mediated radical addition of perfluoroalkyl iodide to alkene in water

PATILKALPESHTUMADU chirumarrysridhar 김한솔 VAIDYARAGHAVENDERRAO 신동수*

창원대학교 화학과

Many fluorinated compounds exhibit unique properties such as thermal and chemical stability, and noteworthy hydrophobicity and lipophilicity. Many studies on synthesis with perfluoroalkyl iodides using several metals as initiators for the radical reactions have already been carried out. The intermolecular carbon–carbon bond formation reactions are initiated by copper, palladium, Raney nickel, etc. and are achieved in organic solvents or organic–water mixture solvents. While intermolecular radical perfluoroalkylation reactions in water have attracted attention in the field of fluorine chemistry, reports of the addition reaction in water are rare. Now we wish to report the addition of perfluoroalkyl iodides to alkenes in the presence of quantitative amounts of iron in water to afford adducts in good yields which would be more convenient, eco-friendly and economical as compared with other methods of perfluoroalkylation of alkenes.


nC4F9I
R
Fe, H2O
50 °C, 30 min
C4F9
I
R
nC4F8I2
R
Fe, H2O
50 °C, 1.5 h
C4F8
I
R
2

R = alkyl

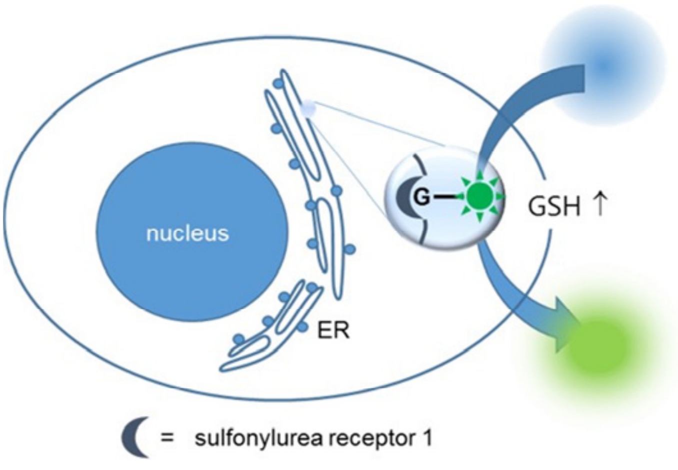
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-358**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

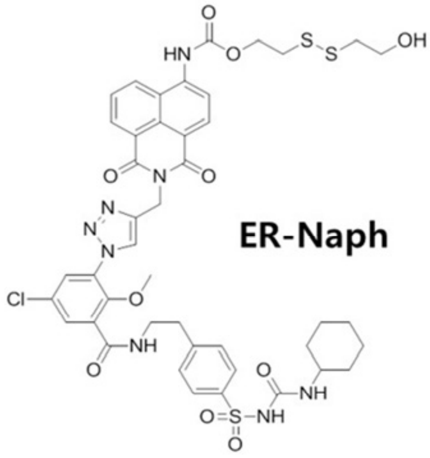
Glibenclamide-mediated Endoplasmic Reticulum Glutathione Sensing

조혜령 이재홍 이은아[1] 강철훈* 김태우*

경희대학교 동서의학대학원 [1]경희대학교 의과학연구원

Endoplasmic reticulum (ER) is primarily responsible for the proper sorting of lipids and proteins, and for the protein folding in cells. Unregulated reactive oxygen species (ROS) generation disrupt the redox balance on ER resulting to an accumulation of misfolded and unfolded proteins, a condition known as ER stress. As a result, the live cell imaging of reductive environment on ER is important to understand ER response under oxidative stress. We synthesized a glibenclamide-mediated, disulfide based ER glutathione sensing probe (ER-Naph). Interestingly, the fluorescence change of ER-Naph in GSH/cytosolic protein extracts was not interfered by Thioredoxin, a well-known disulfide redox protein. Confocal fluorescence microscopy shows the ER targeting of ER-Naph and its reasonable fluorescence response on ER stress. ER-Naph is the first report to detect GSH change at ER location without disulfide reducing protein interference, to our knowledge.





ER-Naph

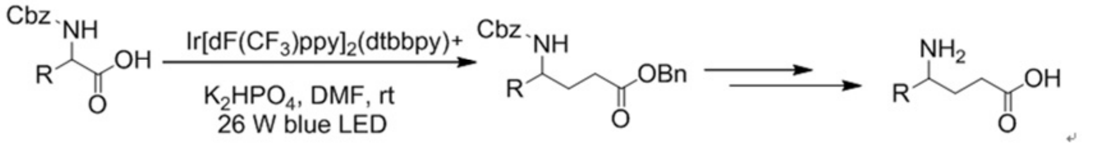
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-359**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of γ-Amino acid from α-Amino acid using iridium photocatalyst under visible blue LED light

<u>PATILKALPESHTUMADU</u> 신동수*

창원대학교 화학과

As we know amino acid is most important for human body functionalization and biosynthesis. The synthesis of γ-amino acid using chemical synthesis are required many step, so in our research we reduced certain step to synthesis of γ-amino acid from α-amino acid using iridium catalyst under visible LED light. This Micheal addition accomplished via decarboxylative activation of amino acid by visible light using photocatalyst activation. Photo-induced oxidation of carboxylic acid including amino acid provides CO2 –extrusion platform to generate Micheal doners without the requirement for organometallic activation.



α-Amino Acid γ-Amino Acid

(R = Aryl. Alkyl)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-360**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Secondary Structure-inspired Design of Small-molecule Modulators for the Study of Unexplored Protein-Protein Interactions

박원우 김찬우[1] 박승범[1,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

In the field of chemical biology, protein-protein interaction (PPI) is a major research topic since it plays a central role in signaling pathway and network in living system. So, the ability to control PPIs is potentially of great significance given that it will allow us to understand biological phenomena deeply, and especially, develop new molecular therapeutics to overcome human diseases. However, despite the importance, the understanding and exploitation of the principle of PPI for developing new drug is still at the early stage. It is known that 2nd structures, such as α-helix or β-strand, on PPI interface are largely involved, with playing recognition roles.Meanwhile, the presence of hot-spot on PPI and peptidomimetic approach makes it amenable to small molecule perturbation on PPI. However, as we know how PPI works very little, it should be beneficial that the library member covers as many of secondary structure as possible in order to explore various type of PPI binding mode. So the mimetic scaffolds are designed to cover three major secondary structures: a-helix, b-strand and b-turn. In addition, the mimetic scaffolds will be synthesized from a single skeleton in a practical mean to construct hundreds-membered library with wide coverage of interacting modes. From the 40-membered virtual library that commonly contains pyrimido-diazepine, suitable candidates were selected by comparing major secondary structures with three to eight sequence long. The selected candidates display analogous shape and residue projection to corresponding secondary structures. Each of three candidates require different building blocks that determines distinct structural characters from each other, but is synthesized by analogous pathways to contain a common molecular framework.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-361**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Immobilization of Organic Molecules on Silica Surface Using Diisocyanate Derivatives

박우진 정희태 전철호*

연세대학교 화학과

Organic-inorganic hybrid materials are interesting materials that have both organic and inorganic character, since these materials have the advantage that overcome individual limit. Mesoporous silica can be used as inorganic material for immobilizing fluorescent organic molecules or bioactive molecules such as enzymes by diisocyanate derivatives. Diisocyanate derivatives are highly reactive electrophiles, which react with a variety of nucleophiles including alcohols, amines and even water. The reaction is carried out by step-by-step immobilization of diisocyanate derivatives onto silanol-group of silica surface and then amino group of organic molecules. Immobilized fluorescent material like N-dansylethylenediamine can be determined by using fluorescence spectrometer and elemental analysis (EA).

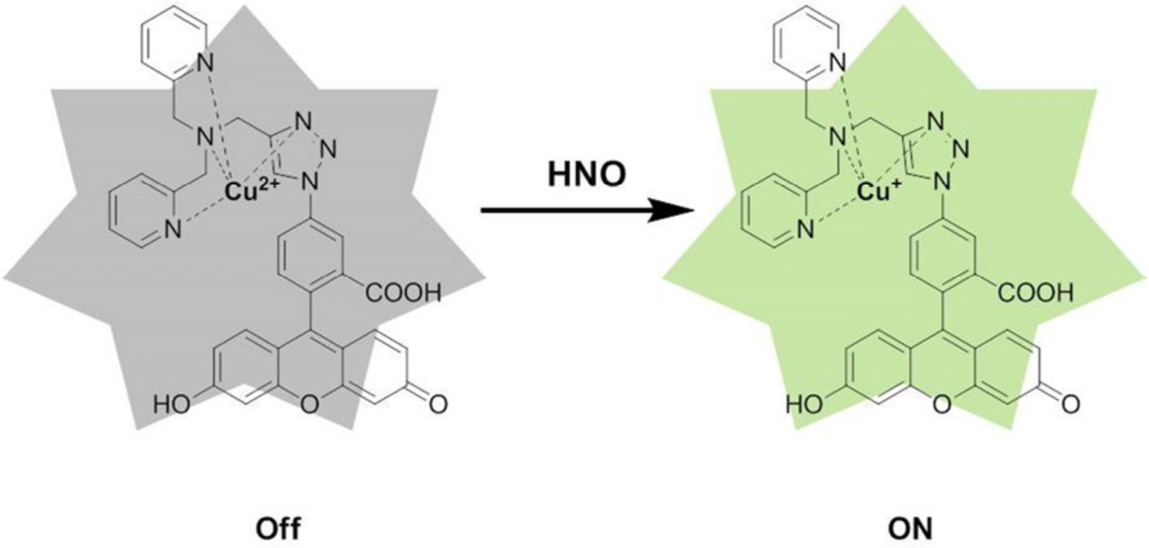
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-362**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Di-(2-pocolyl)amine-fluorescein Click Conjugate As a HNO Fluorescence Probe

이용재 이재홍 강철훈* 김태우*

경희대학교 동서의학대학원

Nitroxyl (HNO) is the one-electron-reduced form of nitric oxide (NO). HNO displays distinct responses under diversity of biological conditions, such as superoxide or free thiol scavenging. Already several groups reported fluorescent HNO probes, but a few arguments remind on the action mechanism and in vivo imaging of the probes. Thus we synthesized a new di-(2-pocolyl)amine-fluorescein click conjugate as a HNO fFluorescence probe. The probe showed selective binding for copper (II) ion and the probe's fluorescence was quenched after binding copper (II). The quenched fluorescence of copper (II)-fluorescein complex was selectively recovered by HNO in various reactive oxygen species and reactive nitrogen species.



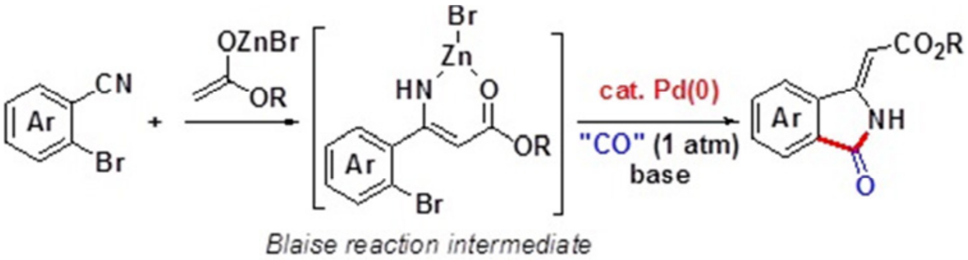
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-363**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Tandem One-pot Synthesis of (Z)-3-Methyleneisoindolin-1-ones through Pd-Catalyzed Aminocarbonylation of the Blaise reaction Intermediate

XUAN ZI 이상기[1,*]

이화여자대학교 화학.나노학과 [1] *이화여자대학교 화학/나노과학과*

The 3-methyleneisoindolin-1-one moiety represents a structural subunit in numerous natural and synthetic products that exhibit a wide range of biological activities. Many reliable methods have been developed for the preparation of 3-methyleneisoindolin-1-ones. However, these methods suffer from poor E/Z stereoselectivity of the methylene moiety. In the course of our ongoing study on tandem use of the Blaise reaction intermediate, we have developed various transformations of nitrile into N-heterocyclic compounds.1 Recently, we reported palladium/solvent controlled divergent catalysis of Blaise reaction intermediate with an excellent compatibility with transition metal catalyst.2 Based on these research, we have developed a tandem palladium-catalyzed aminocarbonylation of Blaise reaction intermediate with carbon monoxide (1.0 atm), giving isoindolin-one derivatives. This protocol provides mild reaction conditions, operation simplicity, good functional group tolerance and high product generation.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-364**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Anisotropic thyminated foldecture from β-peptide foldamer

오병창 이희승*

KAIST 화학과

Due to its rigid secondary structure as well as rapid interactions between molecules, self-assembly of foldamer can yield unique-shaped three-dimensional (3D) microstructure called foldecture. Especially trans-(S,S)-2-aminocyclopentanecarboxylate hexamer (ACPC6) has sufficiently long peptide length to maintain high 12-helix stability, reporting both protected and deprotected C-terminal forms assembled to foldectures with high homogeneity.1-2 The mechanism of the self-assembly to foldecture, which mainly depends on non-covalent interaction between the helices, suggests the way to functionalize the foldecture surface. Typical foldectures have polyhedral 3D structure with asymmetrical facets due to ordered packing of foldamer building blocks throughout the foldecture body. Therefore, introduction of a functional moiety at the peptide terminus would make the assembled foldecture exposing the moieties only on the specific facet, i.e. functionalize the foldecture anisotropically. Nucleobase thymine has chosen as the suitable group, since it has selective hydrogen-bonding ability with its complementary base adenine and therefore can be conjugated with biomolecules (e.g. polynucleotide ends with polyadenine). Herein, we report self-assembly of a C-terminal thyminated ACPC6 foldamer (Boc-ACPC6-Thy) and molecular packing structure of the foldecture. The obtained foldecture has homogeneous rhombic rod shape with the adopted thymine groups heading one direction, with a thoroughly different molecular packing aspect from the precedent ACPC6-based foldectures. The surface characteristic of the novel foldecture can be applied as an organic platform for biomolecular sensor or probe.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-365**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Construction libraries of triazole hybrid molecules and its application to autophagy modulator and ALS model

김민지 정진주[1] 박승범*

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

1,2,3-Triazoles have received much attention, as their intriguing physical and biological properties as well as their excellent stability render them promising drug core structures. They have wide coverage of biological applications including anticancer,antibacterial, anti-inflammatory and antimalarial activites and are also useful synthetic intermediates in small molecules. Also, 1,3-dipolar cycloaddition is an efficient tool that facilitates the formation of heterocyclic bridges between the different units to couple them together. To club the privileged scaffold with other diverse aryl substituent, we utilized triazoles as the bridging mediator via 1,3-dipolar cycloaddition. Therefore, we constructed the libraries of triazole hybrid molecule by the click reaction. As a next step, the compounds of triazole libraries were screened using lipid droplet screening method which is a phenotypic and cell image-based assay in living cells to identify active compounds that can induce autophagy without causing cytotoxicity. Autophagy is a major clearance and pro-survival pathway for recycling cytoplasmic components and for the removal of aggregated proteins, organelles, and lipid droplets by lysosomal degradation. The western blot of LC3 and p62 was also confirmed in NSC-34 motor neuron cells, which are responsible for the degradation of mutant supreroxide dismutase1(SOD1) and the degradation of mutant SOD1 aggregates in presence of the hit compound was observed in real-time monitoring system. In the result of in vivo study, the hit compound substantially extended lifespan of C.elegans expressing SOD1-G85R and the extension was specific for the mutant SOD1. This study will be informative for the growing field as research tools and developing drugs for autophagy-related diseases.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-366**

발표분야: 유기화학

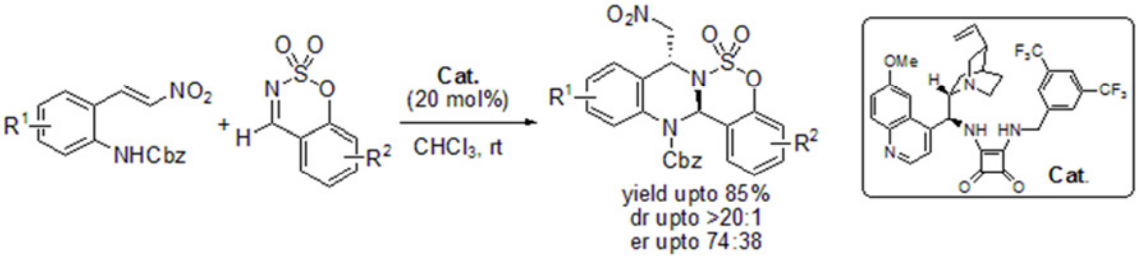
발표종류: 포스터, 발표일시: 금 11:00~12:30

Stereoselective synthesis of benzosulfamidate-fused tetrahydroquinazoline via organocatalytic imine addition/aza-Michael cascade reaction

심종택 김성곤*

경기대학교 화학과

A concise synthetic route to valuable highly functionalized benzosulfamidate-fused tetrahydroquinazoline is presented. The imine addition/aza-Michael cascade reaction of *N*-Cbz-2-amino-β-nitrostyrene and benzoxathiazine 2,2-dioxide using an imidazole as catalyst afforded tetrahydroquinazolines with high diastereoselectivities. And chiral quinine-derived squaramide organocatalyst promoted an asymmetric cascade reaction to provide enantioenriched benzosulfamidate-fused tetrahydroquinazoline with good enantiopurities (up to 74:38 er).



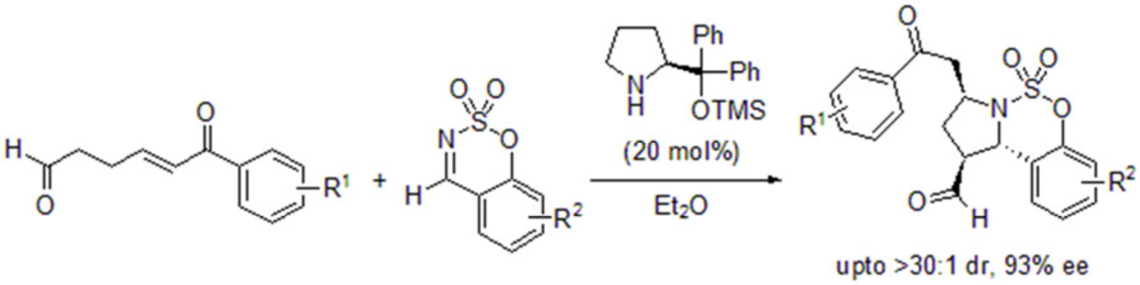
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-367**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Organocatalytic enantioselective cycloaddition of δ-formyl-α,β-unsaturated ketones with cyclic N-sulfimines: Construction of chiral highly functionalized sulfamidate-fused pyrrolines

김한나 김성곤*

경기대학교 화학과

A highly efficient asymmetric synthesis of sulfamidate-fused pyrrolines utilizing organocatalysis has been developed. The asymmetric organocatalytic imine addition/aza-Michael cascade reaction domino reaction of δ-formyl-α,β-unsaturated ketones with cyclic *N*-sulfimines using a diphenylprolinol TMS ether as an organocatalyst afforded the corresponding highly functionalized sulfamidate-fused pyrrolines good yields and with high levels of stereoselectivities (up to >30:1 d.r., 93% ee).



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-368**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Cytoxicity test and synthesis of Hexahydro-1,3,5-triazines

박지송 정대일* 이도훈 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Hexahydro-1,3,5-triazines are reduced derivatives of 1,3,5-triazines and the parent triazines, they are conformationally flexible. N-substituted 1,3,5-triazacyclohexanes are an important class of heterocycles due to their versatile use in the coordination chemistry, catalysis, switchable system with light or redox trigger, crown ether system as well as in recognition, extraction and detection requiring molecular selectivity. Classical Mannich synthesis of 1,3,5-trisubstituted-1,3,5-triazines is accomplished by the condensation reaction between formaldehyde and amine. However, these methods suffer from disadvantages such as harsh conditions, unsatisfactory yields and long reaction time. In this study, we attempted the synthesis of 1,3,5-trisubstituted-1,3,5-triazines in order to obtain novel compounds with biological applications in high yields. Cytotoxicity test of synthesized 1,3,5-trisubstituted-1,3,5-triazines was performed at medical center of Dong-A University

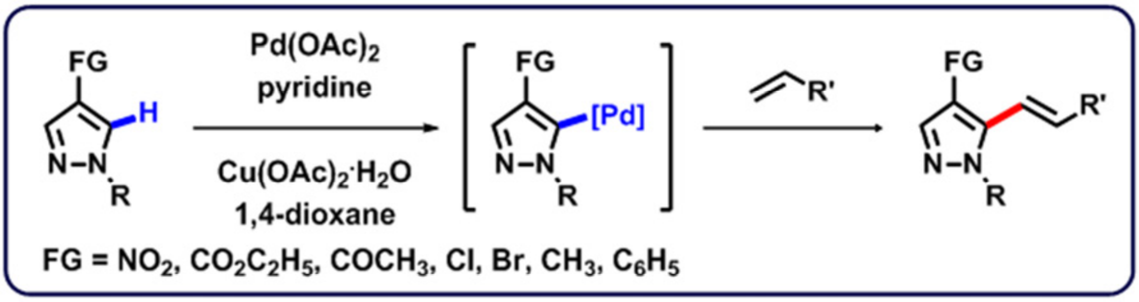
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-369**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

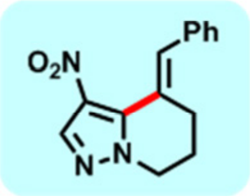
Pd Catalyzed Direct C−H Alkenylation of Pyraozles

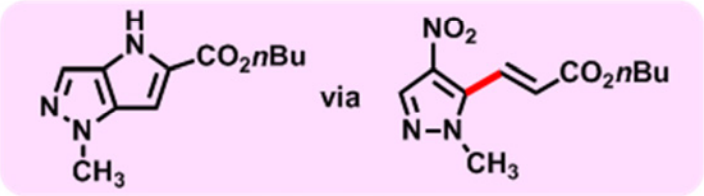
김현태

부산대학교 화학과

We have developed inter- and intramolecular C−H alkenylation reactions of pyrazoles. The catalyst, derived from Pd(OAc)2 and pyridine, enabled the oxidative alkenylation of pyrazoles containing a variety of functional groups at the C4 position. Activated alkenes, including acrylate, acrylamide, and styrene derivatives, and enamides could be installed in this process. The sequential C−H alkenylation and cyclization reactions gave rise to fused bicyclic pyrazoles, providing a new strategy to annulate readily available pyrazole compounds.







일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-370**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of fluorescent mitochondria probe based on 1,2-dihydro-3H-pyrrolo[3,4-b]indolizine-3-one

성준 김은하* 차정현[1]

아주대학교 분자과학기술학과 [1]아주대학교 응용화학생명공학과

One of the most important eukaryotic cellular organelle, mitochondria have various size, and number depends on the condition of the cells. Mitochondria take critical roles in our body. Mitochondria make ATP with oxidative phosphorylation process in mitochondrial inner membrane. Futhermore mitochondria also control cellular signaling, apoptotic cell death and redox homeostasis. They are polymorphous organelles having versatile structural differences depending on cell type, cell-cycle and intracellular metabolic state. Therefore, there are high demands for fluorescent probes can monitor mitochondrial morphology and it will be useful for high contents screening and molecular diagnostic tools for the diseases. 1,2-dihydro-3H-pyrrolo[3,4-b]indolizine-3-one (Seoul-Fluor) can be used as molecular platform to systematically generate the versatile fluorophores having different photophysical properties. In this context, our research group planned to make fluorescent mitochondria probe utilizing Seoul-Fluor system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-371**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Structure photophysical property relationship study about indolizine core

최상기 김현기 김은하*

아주대학교 분자과학기술학과

To understand basic biology and to develop therapeutics for curing the disease, fluorescent imaging technique has become an inevitable scientific tool for investigating biological system in basic research and clinic. Many strategies have been pursued to develop new fluorescent bioprobe for the technique, which can specifically visualize specific cell type, cellular state or biological markers. Our research team hypothesized understanding about structure photophysical property relationship about fluorescent pharmacophore can boot up the speed for discovery of versatile fluorescent bioprobes against multiple different bio-markers. Indolizine, one of the five isomers of indole, is a well known pharmacophore of multiple different alkaloids and their synthetic derivatives have been found to exhibit a variety of biological activities. Interestingly a few derivatives of this 10π electron conjugated planar electronic structure have fluorescent properties. Therefore we believe indolizine core skeleton can be used as fluorescent pharmacophore and systematic study can unveil the relationship between chemical structure and photophysical properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-372**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Design and synthesis of new mass tags for matrix-free laser desorption ionization mass spectrometry (LDI-MS) based on imidazo[1,2-a]pyridine

김태겸 문봉진*

서강대학교 화학과

Matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF-MS) is widely used in analyses of biomolecules such as proteins and peptides.[1] Also, MALDI-TOF-MS has been used in various clinical diagnostic applications as well.[2] In this technique, the sample is detected by MALDI-TOF-MS with various matrices which assist the ionization of analyte on laser irradiation. However, these matrices can contaminate the mass signals in the low molecular weight region. To avoid this problem, a new technique called matrix-free laser desorption ionization mass spectrometry (LDI-MS) was developed, where heterolytically photocleavable mass tags were employed under matrix-free conditions. We have designed and synthesized new mass-tags based on imidazo[1,2-a]pyridine structure that can be photochemically ionizable upon UV-irradiation. In our experiments, when the mass-tag was exposed to UV light, methoxy group or mercaptopropionic methyl ester group were detached. And then, conjugated mass-tag fragment ion signals can be detected without aid of matrix under LDI-MS conditions. After chemical conjugation of mass tags with biomolecules such as peptide, UV laser irradiation selectively generated the corresponding mass-tag fragment ions. By using these technique, multi-detection of biomolecules will be capable with substitution of alkyl groups on imidazo[1,2-a]pyridine backbone in a different position. The tags were easily synthesized in 3 steps and in considerably high overall yields (30-50%) starting from commercially available starting materials.

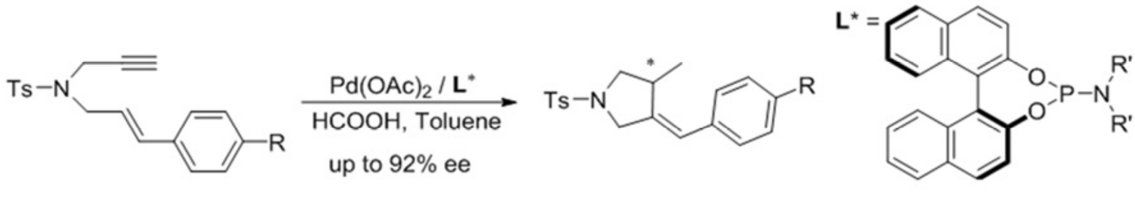
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-373**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Palladium Catalyzed Enantioselective Cycloreduction of 1,6-Enynes by Use of Chiral Phosphoramidite Ligands

박희건 한진욱* 오창호*

한양대학교 화학과

The cyclization of enynes has been widely utilized in the synthesis of structurally complexed natural and synthetic product. Asymmetric cycloreduction of 1,6-enyne by palladium catalysts coordinated with chiral monodentate phosphorus ligand, especially phosphoramidites, in the presence of formic acid will give optically active cyclized organic compounds from a wide variety of conjugated enynes.Herein, we wish to report that a Pd-catalyzed asymmetric cycloreduction of various 1,6-enynes by use of chiral phosphoramidite ligands. The reactions proceed smoothly at 60 °C with $Pd(OAc)_2$ (5 mol %), chiral ligand (10 mol %), and formic acid (1.7 equiv) as a reductant in toluene with high catalytic activity and enantioselectivity (up to 92% ee).Chiral phosphoramidite ligands prepared from (*S*)-1,1'-binaphthol and various secondary amines were examined in order to evaluate the influence of secondary amine part of the phosphoramidite ligands in enantioselectivity.



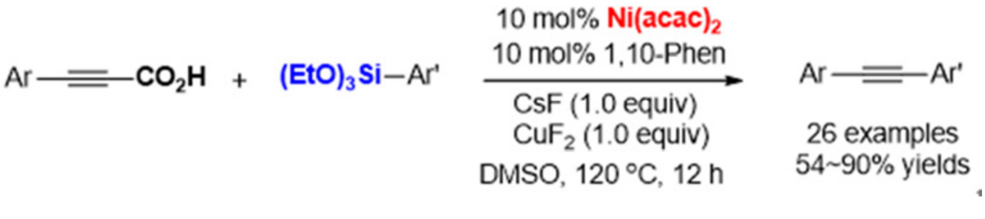
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-374**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Decarboxylative Coupling Reaction of Propiolic Acids with Organosilanes using Nickel Catalyst

GABRIELCHARLESEDWINRAJA JAYARAMAN ARAVINDAN 이선우*

전남대학교 화학과

In recent decades, low-cost metals are being explored in transition-metal catalyzed reactions. Ni catalytic systems have been less developed compared to Pd for coupling reactions even though Ni is less expensive. Decarboxylative cross-coupling reactions have been studied in detail using various coupling partners such as iodides, bromides, and chlorides; benzyl halides have also been used. However, organosilane compounds have never been used as the coupling partner in decarboxylative coupling reactions with alkynyl carboxylic acids, even though they have several advantages such as storage and handling because of their good stability.Recently, we developed a Ni catalyzed decarboxylative coupling reaction of alkynyl carboxylic acids with organosilanes as the coupling partner for the first time. Ni(acac)2 and 1,10-phenanthroline showed the best result in the presence of CsF and CuF_2 at 120 °C. This system tolerated the presence of alkyl, alkoxy, halogen, nitro, cyano, ketone, and ester functional groups. Moreover, the reaction with but-2-ynedioic acid and organosilane afforded the corresponding symmetrical diarylalkynes.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-375**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Propargyl alcohols via Transition Metal-Free Decarboxylative Coupling Reaction of Aryl alkynyl carboxylic acids

IRUDAYANATHANFRANCISMARIARAJ 김한성 이선우*

전남대학교 화학과

Propargyl alcohols are vital structural units in bioactive compounds. Literature precedents shows various synthetic methodologies for the preparation of propargylic alcohols. The reaction between terminal alkynes and either aldehydes or ketones is one of the most frequently used methods, employment of a strong base such as alkyl lithium, dialkyl zinc, or organomagnesium reagent was required to activate the terminal alkyne hence, these methods have the disadvantage of a narrow scope of substrates. In addition, transition metal catalysts have also been employed in the reaction between terminal alkynes and aldehyde/ketones for the formation of propargyl alcohols.We have developed a direct synthesis of propargyl alcohols from the reaction with a variety of aryl propiolic acids and aldehydes/ketones in the absence of a transition metal catalyst. In the presence of Cs_2CO_3, the desired propargyl alcohols were formed in good yield. The methodology was also extended to the reaction with 2,2,2-trifluoroacetophenone which afforded the trifluoromethylated propargyl alcohols in good yield. To the best of our knowledge, metal-free conditions have not been reported in the decarboxylative alkynylation of trifluoromethyl ketones. We found that the decarboxylative coupling reactions with alkynyl carboxylic acids showed high yield than the reaction with terminal alkynes in the formation of propargyl alcohols.

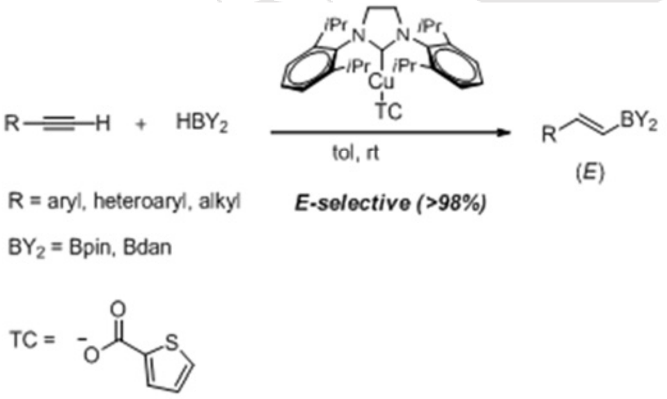
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-376**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Well-defined Carbene-copper Complex-catalyzed Hydroboration of Terminal Alkynes

장원준 김남현 장수연 윤재숙*

성균관대학교 화학과

Boron addition to alkynes provides an efficient synthetic method of useful alkenylboron intermediates in organic synthesis. In this presentation, we report an highly regio- and stereoselective synthesis of alkenylboron compounds from terminal alkynes through copper-catalyzed hydroboration. Using an air stable and well-defined carbene-copper(I) complex, various (E)-alkenylboron compounds were produced with pinacolborane and 1,8-naphthalene-diaminatoborane without any base.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-377**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Structural Analysis of Foldamers Featuring a Cyclopropyl Amide in N-terminus

임다님 이희승*

KAIST 화학과

Hydrogen bond plays an important role in maintaining the structural integrity of large-scale biological structures such as ribonucleotide helices and enzymes.1 Although the importance of conventional N-H•••O hydrogen bonding is fully appreciated, far less is known about C-H•••O hydrogen bonding and surprisingly, C-H•••O hydrogen bonding has never been investigated in the context of foldamer self-assembly. In this study, we described the design, synthesis, structural characterization and self-assembly behavior of new foldamers that contain a structural motif – an N-terminus cyclopropyl amide – known to participate in bifurcated NH•••O/CH•••O hydrogen bonding.2 A series of 11-helical α/β-heterogeneous backbone foldamers were used as a backbone and coupled with cyclopropane carboxylic acid using standard solution-state peptide synthesis methods. Structural analysis of these foldamers were then accomplished through 1D NMR spectroscopy, CD spectroscopy and single-crystal X-ray crystallography. Although the differences in the unit cell of the foldamer, consistence in intermolecular hydrogen bonding pattern were found in the single-crystal X-ray structures. This shows that cyclopropyl amide motif might be use as a synthon that could control the molecular self-assembly.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-378**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient synthesis of methopholine through double addition of alkyl halides on dihydroisoquinoline

김슬기 **AcharyRaghavendra**[*] **Gangadhar Rao Mathi**[*] 황종연[*] 윤창수[*] 김필호[*]

한국화학연구원 의약화학연구센터

Tetrahydroisoquinoline (THIQ) and dihydroisoquinolines (DHIQ) scaffolds are one of the major structural motifs in pharmaceutical compounds as well as natural products. During the course of studies toward the synthesis of diverse THIQ, double addition of alkyl halides on 1-methyl-3,4-DHIQs (MDHIQ) was discovered, one at the amine the other at the C1-methyl group of MDHIQ. It turns out that diverse alkyl halides and DHIQs were compatible for this reaction. Moreover, two different kinds of alkyl halides could be sequentially introduced to MDHIQ in one-pot reaction. The application of this unique chemistry to the total synthesis of a natural product, methopholine, was accomplished in just two steps starting from a DHIQ precursor.

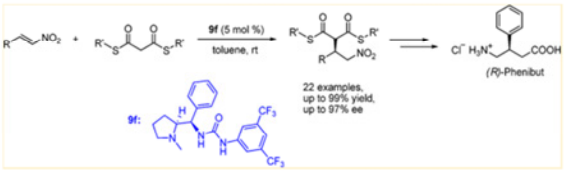
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-379**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enantioselective Conjugate Addition of Dithiomalonates to trans-β-Nitroolefins Catalyzed by L-Proline-Urea Organocatalyst

JINHUI 김승태 강기태 신성호 심수용 김태형 남동국 김재연 조수민 류도현*

성균관대학교 화학과

A series of novel L-proline derived tertiary amine bifunctional organocatalysts are reported, which were applied to the asymmetric conjugate addition of dithiomalonates to trans-β-nitroolefins. The reaction proceeded in high yields (up to 99%) with high enantioselectivities (up to 97% ee). The synthetic utility of this methodology was demonstrated in the short synthesis of (R)-phenibut1 which is a therapeutically useful agonist of γ-aminobutyric acid (GABA) type-B receptors and is used as a neuropsychotropic drug.2



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-380**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A New Type of Proton Donor using Bronsted Acid Assisted Lewis Acid Catalyst : Enantioselective Insertion of Diazocompounds into O-H Bonds of Benzoic Acid

강기태 김승태 신성호 심수용 JINHUI 김태형 남동국 김재연 조수민 류도현*

성균관대학교 화학과

The asymmetric O-H insertion reaction is an ideal synthetic strategy for preparing optically pure R-alkoxy, R-aryloxy, and R-hydroxy carboxylic acid derivatives, which are valuable building blocks for the construction of natural products and other biological active molecules. In this presentation, A new type of chiral proton donor which is combined with Brønsted acid–assisted chiral Lewis acids (chiral BLAs) and carboxylic acid will be discussed. This new chiral proton donor is highly effective reagent for enantioselective protonation and O-H insertion. The reaction proceeded in good yields (up to 97%) with excellent enantioselectivities (up to 99% ee).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-381**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of UV absorption-based linker for quantitative analysis of immobilized organic compound on solid surface

최라영 이창희 전철호*

연세대학교 화학과

Quantitative analysis of immobilized organic molecules on solid surface is important since no decisive way of measuring the amount of organic molecule in organic-inorganic hybrid materials. In this report, preparation and application of organic coupling linker containing UV sensitive organic functional group such as coumarin and diazo derivatives are described. By measuring UV absorbance of linker, amount of linker can be readily determined. Likewise, loading rate of immobilized linker onto silica surface can be readily measured by measuring UV absorbance. Based on the calibration curve between absorbance and loading rate of linker determined by elementary analysis of hybrid material, amount of loading rate of organic linker onto silica can be determined by measuring UV absorbance of linker-immobilized glass surface or silica surface.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-382**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Formal Synthesis of Prostaglandin Derivatives

김태형 심수용 김재연 강기태 신성호 JINHUI 남동국 김승태 조수민 류도현*

성균관대학교 화학과

Cardiovascular diseases (CVDs) are the leading cause of mortality. According to the World Health Organization (WHO), 17.5 millions of people died from CVDs in 2012. It occupied 31% of cause of worldwide human deaths and 50% of adults. Various drugs for treatment of CVDs are developed and share large portion of pharmaceutical market. Human body secretes powerful vasodilator itself known as prostacyclin. This molecule strongly inhibits blood clot formation which following platelet activation. Since powerful action of prostacyclin in human body, synthetic prostacyclin sodium salt is available as epoprostenol. Epoprostenol is use for direct vasodilation of pulmonary and systemic arterial vascular beds.Prostacyclin has short life time due to the chemically unstable structure of enol ether moiety and enzymatic degradation. Various metabolites of prostacyclin are identified; these metabolites are exhibit vasodilation activity.Meese group reported synthetic method for 2,3-Dinor-6-keto-PGF1α from Corey's lactone. Our research group interested the intriguing formal total synthesis of prostaglandin and prostacyclin for medicinal chemistry purpose. Development of a modular synthesis of them is essential to access this goal.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-383**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile Synthesis of Acid Chloride by FeCl3-Catalyzed Chlorination of Carboxylic Acid using α,α-Dichlorodiphenylmethane

이수민 민별하나[1] 전철호[1,*]

연세대학교 이과대학 화학과 [1]연세대학교 화학과

Carboxylic acid derivatives are commonly prepared by reacting of acid chloride with various nucleophiles such as alcohol, amine, etc. Therefore, since acid chloride is important intermediate reagent for this purpose, chlorination of carboxylic acid has been widely used in organic synthesis. However, most chlorination reagents are oxalyl chloride, thionyl chloride, phosphorous pentachloride, which has shortcomings like handling problem due to corrosiveness and toxicity. Thus we have tried to find new catalytic chlorination method which can be carried out under very mild condition. And we found that α,α-dichlorodiphenylmethane is a good chlorinating reagent for carboxylic acid. In this reaction, FeCl3 catalyzes chlorination of carboxylic acids to form acid chlorides using α,α-dichlorodiphenylmethane as a chlorine source. Determination of amount of chlorination is measured by making acid derivatives from acid chloride with various nucleophiles.

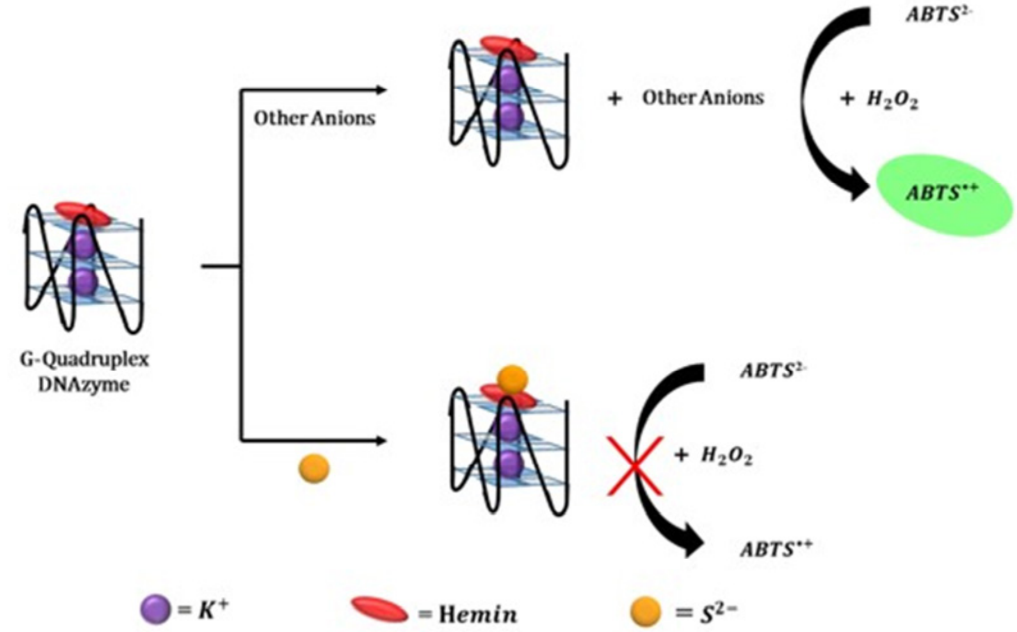
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-384**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

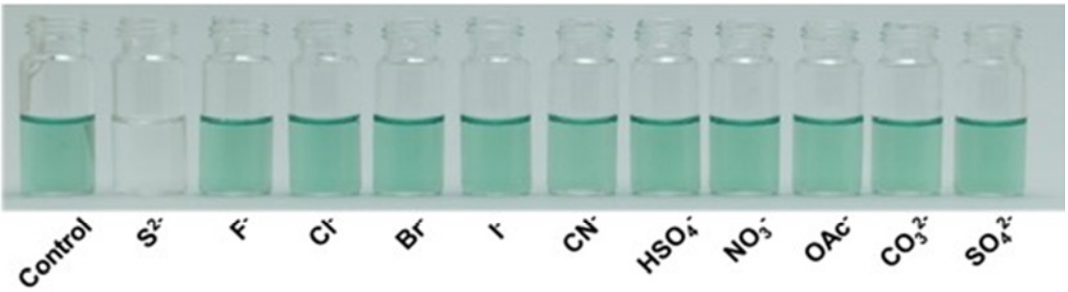
A colorimetric sensor for sulfide detection using direct inhibition of active site inG-quadruplex DNAzyme

오진영 강승윤 한민수*

GIST 화학과

Because of the toxicity of sulfide and its important role in various physiological processes, the development of a selective and sensitive sulfide sensing method is vital. In this study, a colorimetric method for sulfide detection was developed by exploiting the direct inhibition of active site in G-quadruplex DNAzyme by sulfide. Sulfide inactivates the peroxidase-like activity of PS2.M-hemin G-quadruplex DNAzyme by directly blocking the active site of the DNAzyme, allowing the label-free colorimetric detection of sulfide by the naked eye by using 2,2'-azino-bis(3-thylbenzothiazoline-6-sulfonic acid) diammonium salt ($ABTS^{2-}$) as a peroxidase substrate. From titration results, the detection limit of this colorimetric sulfide sensor was estimated to be 412 nM. In addition, the sensor is highly selective for sulfide over various anions and was used to determine sulfide concentrations in tap water samples.


Other Anions
+ Other Anions
ABTS^{2-}
+ H_2O_2
ABTS$^{\bullet+}$
G-Quadruplex DNAzyme
ABTS^{2-}
+ H_2O_2
ABTS$^{\bullet+}$
= K^+
= Hemin
= S^{2-}


Control
S^{2-}
F^-
Cl^-
Br^-
I^-
CN^-
HSO_4^-
NO_3^-
OAc^-
CO_3^{2-}
SO_4^{2-}

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-385**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Low-loading Organocatalytic Synthesis of 3,4-Dihydrocoumarin Derivatives with Adjacent Quaternary and Tertiary Chiral Centers

JINHUI 조수민 김승태 강기태 신성호 심수용 김태형 남동국 김재연 류도현*

성균관대학교 화학과

An L-proline derived thiourea catalyzed Michael addition of 2-oxochroman-3-carboxylate esters to trans-β-nitroolefins is described. This strategy can give direct access to dihydrocoumarin derivatives bearing adjacent quaternary and tertiary stereocenters with up to >99% yield, >20:1 dr, and >99% ee at low catalyst loading (2 mol %). The adduct was further transformed to a spiro-dihydrocoumarin compound in three steps with good yield.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-386**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of A Novel Synthetic Route for Indoloquinolizine Natural Products via Imino-Stetter Reaction

천철홍* 권세현 박은준

고려대학교 화학과

Since natural products bearing an indoloquinolizine scaffold exhibit diverse pharmacological properties and unique chemical structures, these natural products have been considered important target molecules and there have been several synthetic routes to access these natural products. Most common method to access the core structure, indoloquinolizine is Pictet-Spengler reaction between tryptamine and aldehyde. However, these methods generally require relatively lengthy steps.Very recently, our group developed a new method for the synthesis of 2-arylindole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and aldehydes via cyanide-catalyzed intramolecular imino-Stetter reaction.1 We further extended this protocol to the synthesis of indole-3-acetic acid derivatives bearing a pyridyl moiety at the 2-position via imino-Stetter reaction of aldimines from 2-aminocinnnamic acid derivatives and pyridine-carbaldehydes. Subsequent conversion of the carboxylic acid moiety to an alcohol followed by N-alkylation to provide tetrahydro-indoloquinolizine system. Following reduction of the pyridinium ring afforded the expected indoloquinolizine moiety. In this presentation, we will describe our new approach towards the preparation of indoloquinolizine scaffold via cyanide-catalyzed imino-Stetter reaction.Reference1. Lee, S. J.; Seo, H.-A.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 1566.

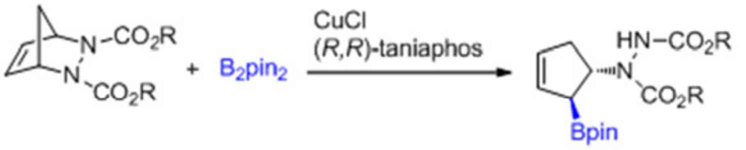
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-387**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Copper-Catalyzed Asymmetric Ring Opening of Diazabicycles with Bis(pinacolato)diboron

이혜수 한정태 윤재숙*

성균관대학교 화학과

We have developed highly enantioselective copper-catalyzed ring opening of diazabicycles with diboron reagent using (R,R)-taniaphos as a chiral ligand. Excellent enantioselectivity up to >99% ee was obtained in the asymmetric ring opening of various bicyclic hydrazines under mild condition, affording 3-bpin-4-hydrazino cyclopentene derivatives. The synthetic utility of the corresponding allylic boron products was demonstrated by various organic reactions. Kinetic resolution of bicyclic oxazine showed the relative rates of C–O and C–N bond cleavage.



up to >99% ee

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

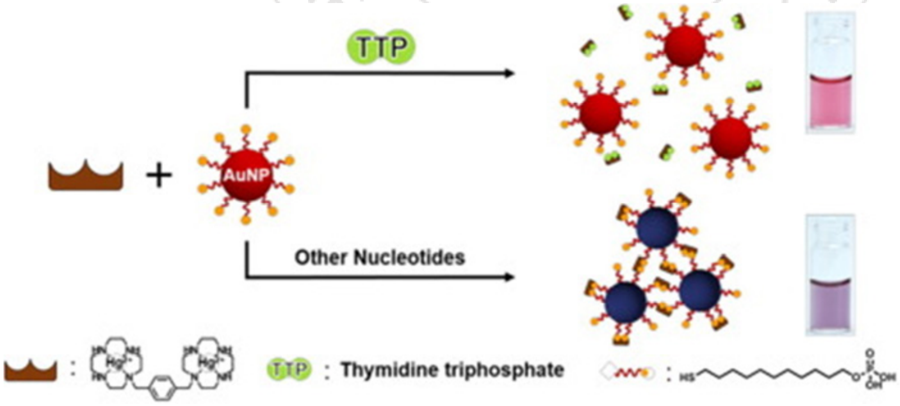
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-388**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of a highly sensitive colorimetric thymidine triphosphate chemosensor using gold nanoparticles and the *ρ*-xylyl-bis(Hg^{2+}-cyclen) complex: improved selectivity by metal ion tuning

유소연 엄민식 강승윤 한민수*

GIST 화학과

In this study, a competitive assay based on a colorimetric sensing system for thymidinetriphosphate (TTP) was developed using 11-mercaptoundecylphosphoric acid functionalizedgold nanoparticles (Phos-AuNPs) and a *ρ*-xylyl-bis(metal^{2+}-cyclen) complex as reporter and receptor units, respectively. A detection limit of 372 nM was achieved with high selectivity for TTP over other nucleotides, including thymidine diphosphate and thymidine monophosphate. The improvement in selectivity was achieved by metal ion tuning in *ρ*-xylyl-bis metal^{2+}-cyclen).



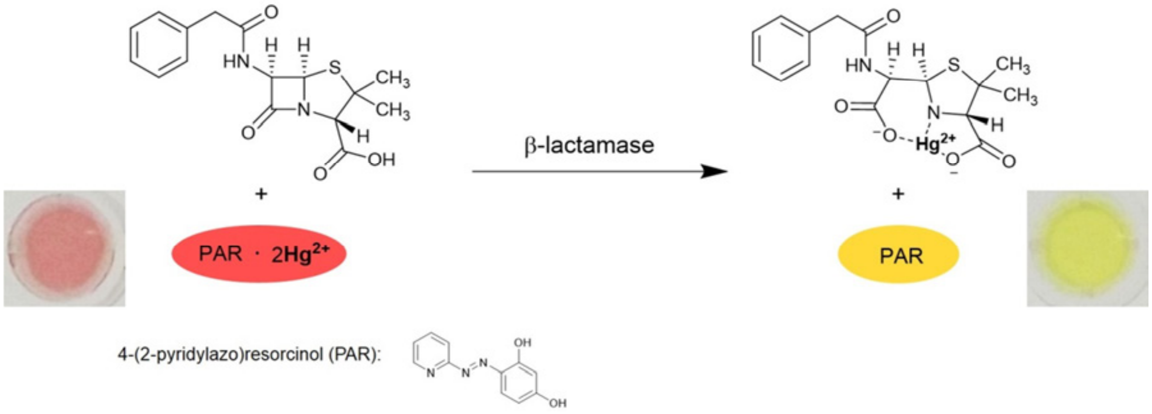
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-389**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Colorimetric assay for β-lactamase activity using cocktail of penicillin and 4-(2-pyridylazo)resorcinol (PAR)-$2Hg^{2+}$ complex

이수지 강승윤 엄민식 한민수*

GIST 화학과

A colorimetric assay for measuring β-lactamase activity and screening its inhibitor was developed using a cocktail of penicillin and PAR-$2Hg^{2+}$ complex. Color change based on the ligand exchange between hydrolyzed penicillin and PAR enabled fast and simple monitoring of β-lactamase activity in real-time. The assay was also applied for high-throughput screening for potent β-lactamase inhibitors.



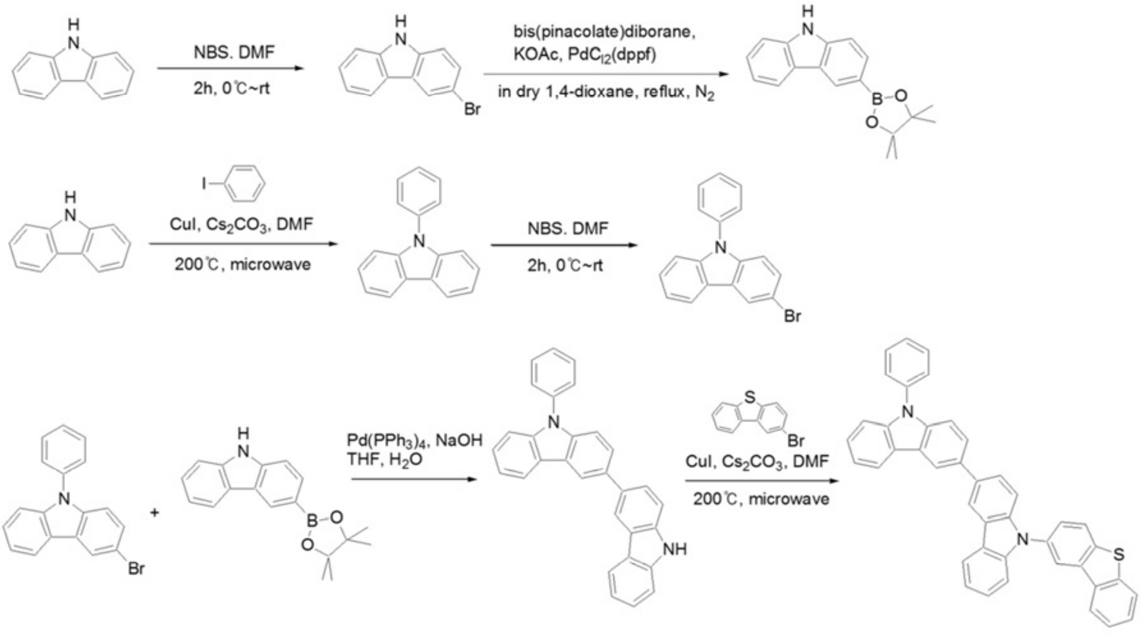
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-390**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of carbazole-dibenzothiophene coupled green host material for PHOLEDs and chracterization of the green phosphorescent device property with FCNirpic

권대련 임춘우[*] 김영관[1,*] 이송은[2]

한남대학교 화학과 [1]홍익대학교 기초과학과 [2]홍익대학교 정보디스플레이공학과

We have designed and synthesized novel carbazole-dibenzothiophene coupled material (BCzDBT) as host material in OLED applications. We used the Spartan 08' program to predict HOMO/LUMO levels and orbital distributions of the carbazole-dibenzothiophene derivative. The synthesized host material was analyzed and confirmed by ^{1}H NMR, ^{13}C NMR, Mass Spectrometer. Also, optical characteristics were examined by UV-vis spectrophotometer and photoluminescence spectroscopy. The thermal stability of host material were analyzed by thermo gravimetric analyzer (TGA) and differential scanning calorimeter (DSC). We have produced a green PHOLED device with FCNirpic and investigated of the device characteristic of BCzDBT based green PHOLED device.


H
N
NBS. DMF
2h, 0℃~rt
H
N
Br
bis(pinacolate)diborane,
KOAc, PdC$_{l2}$(dppf)
in dry 1,4-dioxane, reflux, N_2
H
N
B
O
O
H
N
I
CuI, Cs_2CO_3, DMF
200℃, microwave
N
NBS. DMF
2h, 0℃~rt
N
Br
N
Br
+
H
N
B
O
O
Pd(PPh_3)$_4$, NaOH
THF, H_2O
N
NH
S
Br
CuI, Cs_2CO_3, DMF
200℃, microwave
N
N
S

BCzDBT

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-391**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Molecular design and characterization of host material based on dibenzothiophene for green phosphorescent organic light emitting diodes (PHOLEDs)

안지수 이송은[1] 임춘우[*] 김영관[2,*]

한남대학교 화학과 [1]홍익대학교 정보디스플레이공학과 [2]홍익대학교 기초과학과

Phosphorescent organic light-emitting diodes (PHOLEDs) have been attractive, because theoretical quantum efficiency of phosphorescent emitting material is four times higher than that of fluorescent emitter. Recently, the connection between dibenzothiophene and 9 - phenylcarbazole through 3- position of carbazole was reported to be an effective way of improving the lifetime of the green PHOLEDs.1 High triplet energy electron transport materials with dibenzothiophene cores modified with a diphenyltriazine unit were investigated as electron transport type exciton blocking materials for stable green phosphorescent organic light-emitting diodes.2 In these perspectives, we have designed and synthesized dibenzothiophene-based host materials. DFT calculations were performed using Spartan` 08 software at the B3LYP level. The chemical structures were characterized by ^{1}H-NMR, ^{13}C-NMR, GC-Mass. Thermal stability was analyzed by thermo gravimetric analysis (TGA) and differential scanning calorimetry (DSC). Optical properties of the dibenzothiophene derivatives were analyzed by UV-vis absorption spectroscopy and PL spectroscopy.

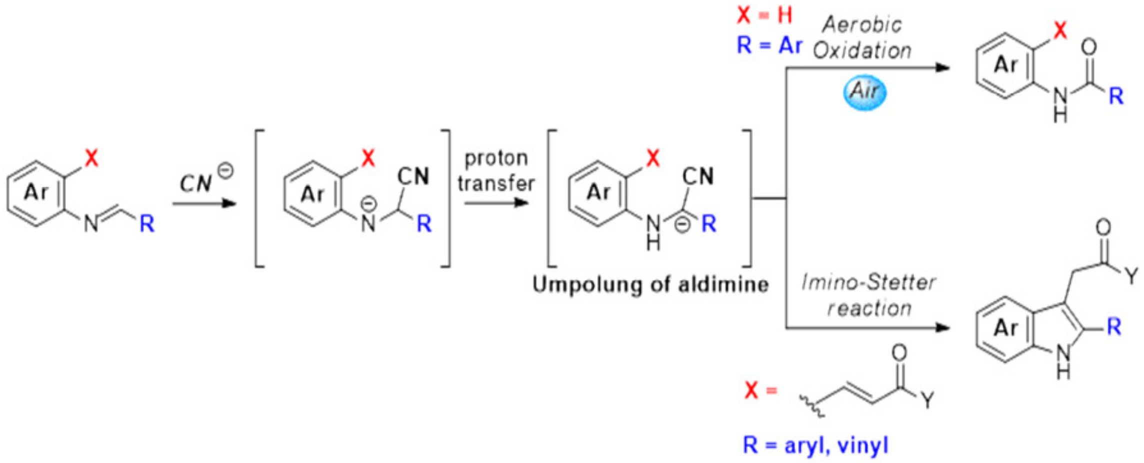
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-392**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of Novel Transformation via Umpolung of Aldimines with Cyanide

천철홍* 서홍안

고려대학교 화학과

Although umpolung reactivity of aromatic aldehydes in the presence of cyanide has been widely utilized in the synthetic community, umpolung reactivity of aldimines with cyanide has been poorly developed. Very recently, we have developed a protocol to convert aldimines derived from aromatic aldehydes and aniline derivatives into the corresponding amides in the presence of cyanide via metal-free aerobic oxidation.1 Mechanistic studies suggested that this aerobic oxidative amidation would be believed to proceed via the addition of cyanide to imines followed by proton transfer from carbon to nitrogen in the original imines leading to umpolung of aldimines, which undergo subsequent oxidation with molecular oxygen in air to provide the desired amide compounds.We further applied the umpolung of aldimines to the synthesis of 2-arylindole-3-acetic acid derivatives with a catalytic amount of cyanide via intramolecular imino-Stetter reaction.2 Furthermore, the application of umpolung of aldimines with cyanide was extended to the preparation of 2-vinylindole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and α,β-unsaturated aldehydes. Various α,β-unsaturated aldehydes could be applied to this protocol and the desired 2-vinylindole-3-acetic acid derivatives were obtained in good yields.3 In this poster presentation, details on the umpolung of aldimines with cyanide and its application to several organic transformations will be discussed. References1. Seo, H.-A.; Cho, Y.-H.; Lee, Y.-S.; Cheon, C.-H. J. Org. Chem. 2015, 80, 11993. 2. Lee, S. J.; Seo, H.-A.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 1566.3. Seo, H.-A.; Cheon, C.-H. J. Org. Chem. 2016, ASAP, DOI:10.1021/acs.joc.6b01621.


X = H
R = Ar
Aerobic Oxidation
Air
CN⊖
proton transfer
Umpolung of aldimine
Imino-Stetter reaction
Ar
X
N
R
CN
N
H
O
Y
X =
R = aryl, vinyl

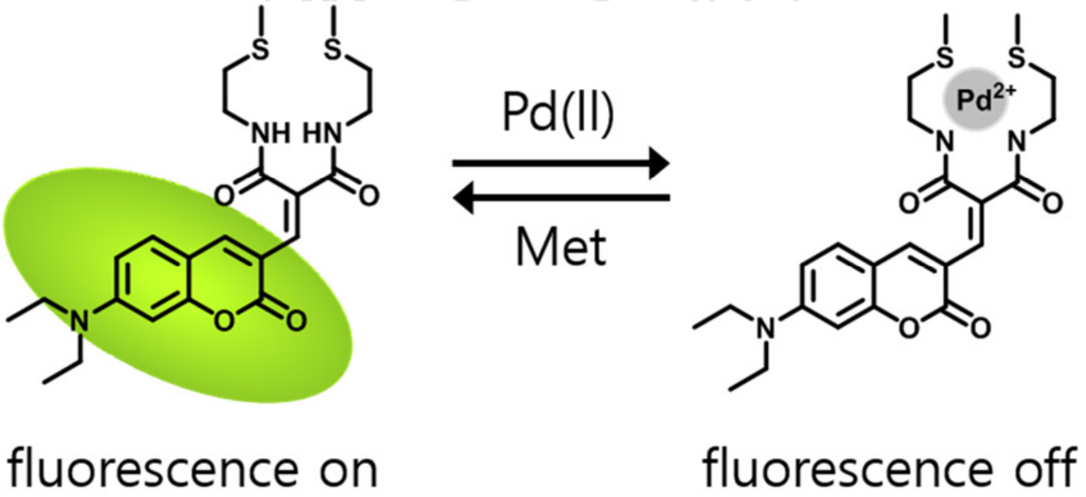
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-393**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dithioether amide based-fluorescent chemosensor for Pd(II) and detection for methionine using its Pd(II) complex

이민아 임태호 한민수*

GIST 화학과

Palladium (Pd) is one of the most widely used heavy metals having importance in industrial fields such as automotive, dental, jewelry and especially in synthetic chemistry. In spite of its usefulness, detection of Pd is essential due to its toxicity that cause health hazard. Herein we suggest dithioether amide based-fluorescent chemosensor enabling simple rapid detection of Pd(II). In contrast to most previous chemosensors for Pd(II) having reaction based mechanism, probe 1 utilizes the binding of Pd(II) to 2-(methylthio)ethylamide moiety of the probe 1 that allows real time sensing. Also, probe 1 showed highly selectivity for Pd(II) over other metals. In addition, 1-Pd(II) complex was applied to detection of methionine using ligand exchange method.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-394**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Direct access to color-tunable fluorescent • •conjugated imidazo[1,2-a]pyridines via palladium-catalyzed C-H amination

이주영

강원대학교 화학과

Imidazo[1,2-a]pyridine, possessing significant and potential biological activities is one of the most widely used N-fused heterocycles. Because of their unique reactivity, many practical synthetic routes for the construction of imidazo[1,2-a]pyridines have been developed. Whereas 2- or 3-arylimidazo[1,2-a]pyridines have received considerable attention, modifications of the pyridine backbone of imidazo[1,2-a]pyridines have been less explored.In this symposium, we will discuss about an efficient method for the construction of synthesize 3,5-diarylimidazo[1,2-a]pyridines through the palladium(II)-catalyzed C-H aminaton of pyridinium zwitterion. In particular, obtained diarylimidazo[1,2-a]pyridines provide an important platform for the design of color-tunable fluorophore by fine tuning the intramolecular charge transfer (ICT) effect.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-395**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Concise Total Synthesis of Paullone via Intramolecular Imino-Stetter Reaction

이상은 이성종 천철홍*

고려대학교 화학과

Paullone, originally known as a class of potent cyclin dependent kinase (CDK) inhibitors, have shown to have various biological activities with further research. The group also acts as inhibitors of mitochondrial malate dehydrogenase (mMHD), and some derivatives, such as kenpaullone (C9-Br) have been reported to target the NAD+-dependent class of histone deacetylases. Additionally, paullone has been reported to have cytotoxic, pro-apoptotic, and antiproliferative characteristics, and is a group that could be valuable for development of medicinal chemistry. Due to these interesting biological activities, paullone has been considered as the target molecule of importance. The usual methods selected are Fischer indole synthesis, transition metal catalyzed coupling, free radical cyclization, and etc. However, most of the former synthetic approaches require long steps. Very recently, we developed a method to synthesize 2-aryl indole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acids and aromatic aldehyde through cyanide-catalyzed imino-Stetter reactions. Since paullone and its derivatives possess a 2-arylindole-3-acetic acid moiety as a common scaffold, we envisaged that paullone could be prepared via imino-Stetter reaction of aldimines derived from 2-aminocinnamic acid derivatives and 2-aminobenzaldehyde. In this presentation, we will describe the synthesis of paullone via imino-Stetter reaction of aldimine from 2-aminocinnamate and 2-nitrobenzaldehyde followed by lactam formation upon reduction of the nitro group with Zn under acidic conditions.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-396**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of Novel Synthetic Routes for Axially Chiral 1,1’-Bi-2-Phenol (BIPhOL) Derivatives

조영인 천철홍*

고려대학교 화학과

Axially chiral biaryl diol derivatives, such as BINOL and VAPOL, have been widely used as either chiral ligands in metal-catalyzed asymmetric catalysis or precursors of chiral Brønsted acid catalysts. Since both substituents and dihedral angles along the chiral axis turn out to play a significant role in the reactivity and selectivity in asymmetric transformation with the biaryl diols, numerous efforts have been made to develop various axially chiral biaryl diol derivatives. However, the effect of dihedral angle has been rather poorly investigated compared to that of substituents; although there are a number of methods for the preparation of axially chiral binaphthol derivatives, such as BINOL or octahydroBINOL, no general synthetic routes for other axially chiral biaryl diols have been developed yet.To address this problem, our group have developed the synthetic pathways of chiral 3,3’-disubstituted 1,1’-bi-2-phenol (BIPhOL) derivatives via diastereomeric resolution using a boronic acid moiety as a resolving group followed by Suzuki-Miyaura reaction.1 In addition, we attempted to develop divergent synthetic routes for other BIPhOL derivatives, such as 1,1’-BISESAMOL, from the same chiral boronic acid intermediate through oxidation of the boronic acid followed by methylenation. However, the desired product was not obtained and unexpected side-product was generated. Alternatively, we developed a route for BISESAMOL through dimerization of sesamol, introduction of boronic acids, followed by diastereomeric resolution using a boronic acid moiety as a resolving group. Subsequent derivatization at the 3,3’-positions allowed us to prepare several BISESAMOL derivatives. In this presentation, we will present the recent progress in the synthesis of axially chiral BIPhOL derivatives.Reference1. Yoon, J.-M.; Lee, C.-Y.; Jo, Y.-I.; Cheon, C.-H. J. Org. Chem. 2016, Under Revision.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-397**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Unexpected gold catalyzed reaction of pyrimidodiazepine derivatives

구재영 박승범[1,*]

서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

Substituted heterocycles are a structural element of a vast number of biologically active compounds. Many studies have been done for development of various heterocycles for over a century, and a variety of well-established methods are available in the literature. Among the many new synthetic transformations, transition metal catalysis has emerged as a powerful tool for various reactions Recently, we have found that gold catalyzed ring transformation pathways are occurred in pyrimidodiazepine derivatives. For example, in the process of our study on the Au catalyzed reaction of pyrimidodiazepine derivatives, we identified imidazolidine derivatives as a major product. Moreover, using different nucleophile from same skeleton, synthesis of oxazolidines could be accomplished. We report herein the details of our study on the Au- catalyzed ring transformation reaction. And also, this gold catalyst reaction exhibited high diastereoselectivity and afforded the highly substituted imidazolidine and oxazolidine derivatives in good yield. The current gold catalyzed ring transformation reaction has not been reported prior to this study.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-398**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rh/Pd synergistic dual catalysis for divergent dipolar cycloaddition reactions from non-dipolar compound

전현지 이상기[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학/나노과학과

The dipolar cycloaddition reactions are among the most useful strategies for the synthesis of substantial variety of heterocyclic compound. But the current dipolar cycloaddition has the intrinsic limitation, which is associated with requirement of at least one dipolar or dipolarphile as a coupling partner. Synergistic dual catalysis system overcomes this limitation. The catalyst converts the non-polar precursor molecule to a reactive dipole that contains the ligated transition metal, which then believed to undergo stepwise dipolar cycloaddition to a stable dipole or a neural dipolarophile to afford a single cycloaddition adduct. So, the development of new strategy from stable non-dipolar compounds is greatly contributed to the synthetic chemistry. Herein, we report the synergistic divergent catalytic cycloaddition reaction between non-dipolar reagent, 1-sulfonyl-1,2,3-triazoles and vinyl ethylene carbamate, obtaining the [3+3] cyclcoaddition adduct and [3+4] cycloaddition adduct selectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-399**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of dihedral angle in donor-π-acceptor dyes for efficient dye-sensitized solar cells

남동국 박준혁[1] 장기태 김승태 김태형 신성호 조수민 심수용 김재연 **JINHUI** 권태혁[2,*] 류도현[*]

성균관대학교 화학과 [1]UNIST 자연과학부 [2]UNIST 친환경에너지 공학부

The Dye-sensitized solar cells (DSCs) have been considered promising candidates for alternative energy systems. We designed and synthesized donor-π-conjugated bridge-acceptor dyes based on indoline, quiloline derivative with planar geometry. Changing planarity and dihedral angle of donor sensitizers, DSC efficiency are affected drastic. investigating these effect, New dyes achieved 9.1% power conversion efficiency at 1.8 μm active layer.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-400**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Cooperative vs. Tandem Catalysis in Rh(II)/Pd(0) Dual Catalytic Transformation of N-Sulfonyl-1,2,3-triazoles

<u>정다정</u> 이규리[1] 이상기[2,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학-나노과학 [2]이화여자대학교 화학/나노과학과

Catalysis is among the most useful and powerful strategies in organic synthesis. When two different catalysts cooperate to run two catalytic cycles concurrently in a catalytic reaction, it creates the opportunity to achieve transformations that would be unattainable with either catalyst alone. However, due in part to the difficulty in ensuring redox-compatibility between the transition metal catalysts, cooperative dual catalysis systems formed by a combination of two transition metal catalysts has been far less explored. Moreover, the mechanistic complexity of these dual catalysis systems has limited the ability to understand these processes. We recent reported that the Rh(II) and Pd(0) catalysts are compatible each other that allow interceptive capturing of π-allyl Pd(II)-complexes, generated from allyl carboxylates or carbonates, with α-imino Rh(II)-carbenoid intermediate, formed with N-sulfonyltriazoles with a Rh(II) catalyst. In present work, we have developed a divergent transformation of triazoles bearing allyl alcohol moiety using Rh(II) and Pd(0) catalysts. Thus, when the reaction was conducted in tandem manner, α-aminoindanone derivatives were produced. In contrast, the mechanistic pathway was altered in cooperative Rh(II)/Pd(0) dual catalytic reaction to afford isoquinolinone derivatives.

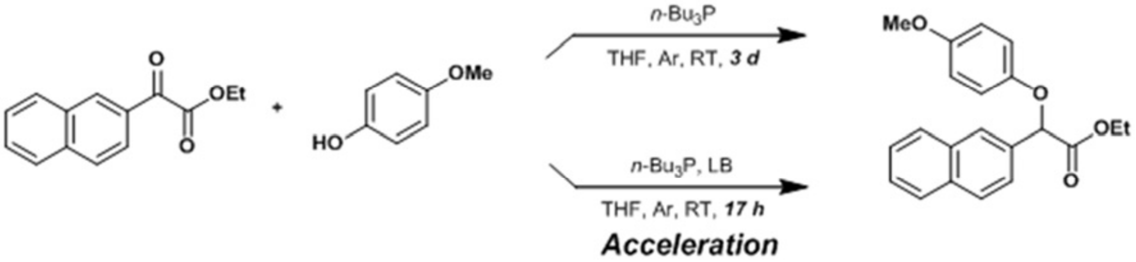
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-401**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Lewis base-catalyzed P(III)-mediated Kukhtin-Ramirez reaction

장한나 정원진*

GIST 화학과

The Kukhtin-Ramirez reaction is P(III) reagent-mediated deoxygenative coupling of 1,2-dicarbonyl compounds with various pronucleophiles. Although the Kukhtin-Ramirez reaction has been known for a while, enantioselective variations are very rare. Recently, an example employing a chiral stoichiometric phosphorus reagent was reported by the Radosevich group. However, a catalytic eantioselective process has yet to be developed. We observed a rate acceleration in the presence of a catalytic amount of Lewis base. Futher investigations with chiral Lewis bases are currently ongoing in order to develop a catalytic enantioselective Kukhtin-Ramirez reaction.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-402**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

C_{60} recognition by 3D-supramolecular network assembly of dimeric copiliar[5]arene and four-way porphyrin derivative

구혜린 김양령 박연실 백경수*

숭실대학교 화학과

The formation of self-assemblies of supramolecular nanolplate by stepwise dimeric copilar[5]arene 1_2, 4-way neutral porphyrin guest 2 and Zn2 were monitored by 1H-NMR and 2D-NOESY experiments. This nanoplate and dipyridyl bridges form 3D-organic supramolecular architectures 3 via quadruple hydrogen bondings, cation-π interactions and metal-ligand coordination. These self-assembled architectures display a remarkable selectivity for the complexation C_{60} within its inner hole which was confirmed by 13C-NMR, UV-Vis spectrometer and HPLC analysis. Especially, the solvent polarity-driven reversible associations and dissociations of fullerene-3D organic supramolecular architectures would enable an easy and efficient separation of fullerenes.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

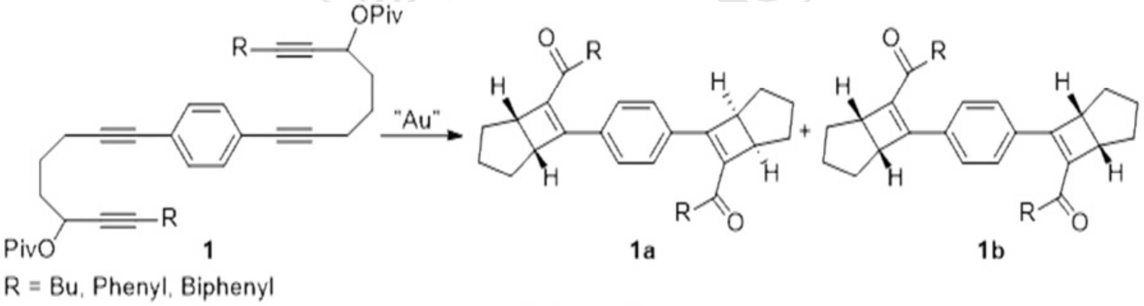
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-403**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of bis(bicyclo[3.2.0]hept-6-en-6-ylmethanone) groups by gold catalyized [2+2] cyclization

김재웅 허훈구 오창호*

한양대학교 화학과

Jaewoong Kim , Hoongu Heo and Chang Ho Oh*Department of Chemistry, Hanyang University, Wangsimni-ro 222, Seongdonggu, Seoul 04763, KoreaWe previously reported gold-catalyzed cyclization of alkyne-propargylic pivaloyl compounds. Propargylic pivaloates could form the allenoate via 1,3-pivaloate rearrangement, which would undergo [2+2] cyclization with the pendent alkyne to give bicyclo[3.2.0]heptenylketone systems. Now, we prepared several substrates which have two alkyne-propargylic pivaloates conjugated with a central system like benzene and naphthalene. These symmetric bis-bicyclo compounds was diastereomeric products and have been separated by using HPLC. We wish to report syntheses and physical properties of these products.



Scheme 1

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-404**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Properties of Boron Difluoride Complex of Annulated Rosarin

이창희* 고유림 **Firmansyah DIKHI** 전민욱

강원대학교 화학과

Ortho-phenylene bridged rosarin (hexaphyrin 1.0.1.0.1.0), known as annulated rosarin is an antiaromatic species with 24 π-electrons. This molecule has unique redox properties upon protonation, while addition TFA and $HClO_4$ yield triprotonated trication rosarin, HI yield an aromatic 26 π-electrons triprotonated monocation rosarin throughout 25 π-electrons of non-aromatic triprotonated monoradical dication rosarin. In continuing our effort to study the redox protonation of annulated rosarin, we synthesized its boron complex to obtain BODIPY types of molecule. Proton NMR and Mass spectra clearly show the formation of one boron complex inside rosarin cavity. UV-Vis spectra shows bathochromic shift on absorption maxima and due to rosarin antiaromatic properties, the BODIPY complex is non-fluorescence. Study on protonation by adding excess of different acids show similarity to parent annulated rosarin, however the study also indicates complex stability on addition of small amount of acid.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-405**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

meso-5,6-Dichlorobenzimidazolyl Calix[4]pyrrole: Displaying High Affinity and Size-Selective Binding Towards Anionic Guests

이창희* **bezaendalemulugeta**

강원대학교 화학과

The anion recognition chemistry of calix[4]pyrroles has been actively studied due to the ubiquitous role of anions in various chemical and biological processes. As a result, many systems have been developed in order to improve affinity and selectivity. Among various model systems, the meso-aryl picket calix[4]pyrroles have been utilized for the selective recognition of anions as well as anion-templated supramolecular capsule formation. With this presentation, a deep cavity calix[4]pyrrole derivatives carrying 5,6-dichlorobenzimidazole units at diametrically crossing meso-positions have been synthesized and fully characterized by spectroscopic means for the first time. The receptor showed high affinity for anions. The additional hydrogen bond donor placed on the meso-substituents play a key role on the enhancement of the binding affinity in addition selectivity of the anions based on their size. The cooperative interaction of anion-pi interactions and hydrogen bonding interaction are thought to be the reason for exceptionally high binding affinity. The detailed guest binding studies obtained from 1H NMR titration, UV-Vis spectroscopy, DFT-calculation data and ITC will be presented in detail.

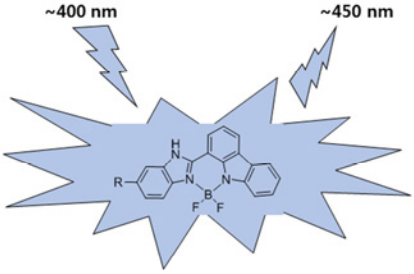
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-406**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Carbazole-based color-tunable BODIPY complexes: Synthesis, structure and photophysical properties

이창희[*] <u>Ranjan Dutta</u> Firmansyah DIKHI 유재덕[1]

강원대학교 화학과 [1]한라대학교 신소재 화학 공학과

Boron dipyrromethene (BODIPY) and its related BF2 complexes have received considerable attention because of their high molecular coefficients and quantum yield values (ΦF), good thermal- and photo-stability, and versatile functionality. Carbazole derivatives have also been studied as potential electron conductors, catalysts, and sensors. Various substituents could be introduced onto the carbazole moiety and effects of substituent could be examined. However, carbazole-based BODIPY dyes showed extensive fluorescence quenching due to intramolecular charge transfer (ICT). Herein we present the synthesis and photophysical properties of a series of carbazole-based BODIPY complexes. In this approach a carbazole-benzimidazole hybrid is generated by condensation of 1-carbazolecarboxaldehyde with 1,2-phenylene diamine moiety. A series of such compounds having benzimidazole groups with various electron withdrawing substituents are synthesized and characterized. Boron complexation of the resulting dipyrrin affords the carbazole-based BODIPYs. These compounds are highly fluorescent both in solution and solid state. Detailed UV-Vis and fluorescence properties and effects of substituents on photophysical properties are examined.


~400 nm
~450 nm
R
H
N
N
B
F
F
N

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-407**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and characterization of self-assembled structures ofdiethylene glycol conjugated β-peptide foldamer

이소망

KAIST 화학과

Biomolecules often assemble spontaneously and organize into higher-order functional nanostructures. To mimic the natural phenomenone, β-peptides were used because of their rigid backbone. Rigidity of foldamer was thought as a critical role for self assembly. However, we wondered that how much it has to be rigid to form foldecture. In this study, we designed and synthesized β-peptide foldamers conjugated with diethylene glycol which has hydrophilicity and flexibility. And surprisingly, we found that a flawed foldamer composed of a bad helix and a totally disordered glycol moiety can make foldectures under the appropriate conditions.

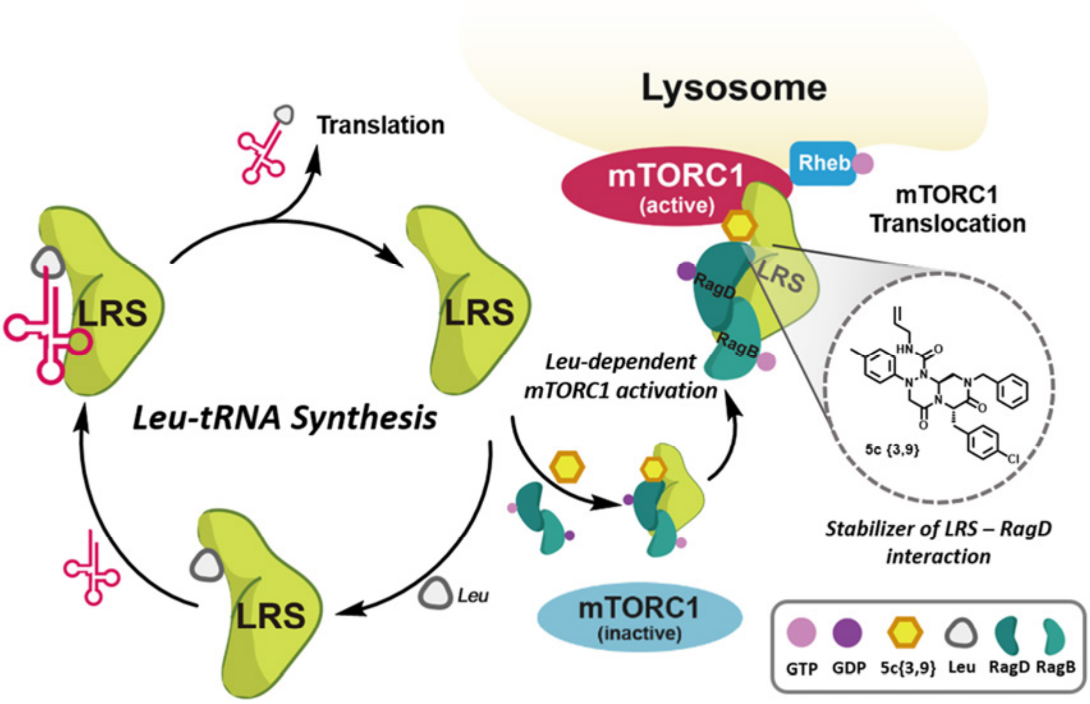
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-408**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

β-Turn mimetic-based stabilizers of protein–protein interactions for the study of the non-canonical roles of leucyl-tRNA synthetase

김찬우 정진주[1] 박승범*

서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과

For the systematic perturbation of protein–protein interactions, we designed and synthesized tetra-substituted hexahydro-4*H*-pyrazino[2,1-c][1,2,4]triazine-4,7(6*H*)-diones as β-turn mimetics. We then devised a new synthetic route to obtain β-turn mimetic scaffolds via tandem N-acyliminium cyclization and constructed a 162-member library of tetra-substituted pyrazinotriazinediones with an average purity of 90% using a solid-phase parallel synthesis platform. Each library member was subjected to ELISA-based modulator screening for the LRS–RagD interaction, which plays a pivotal role in the nutrient-dependent mTORC1 signalling pathway. Western blot analysis of phosphorylated S6K1 as well as FRET-based imaging confirmed that 5c{3,9} stabilizes the direct interaction between LRS and RagD and activates mTORC1 in live cells under leucine-deprived conditions. Thus, 5c{3,9} can be used as a new research tool for studying the non-canonical role of LRS.


Lysosome
Translation
mTORC1
(active)
Rheb
mTORC1
Translocation
LRS
LRS
LRS
LRS
RagD
RagB
Leu-tRNA Synthesis
Leu-dependent
mTORC1 activation
5c {3,9}
Cl
Stabilizer of LRS – RagD
interaction
Leu
mTORC1
(inactive)
GTP
GDP
5c{3,9}
Leu
RagD
RagB

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-409**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of alkyl chain in the supramolecular assembly with SWNT and its electrocatalytic application

장재규 홍종인*

서울대학교 화학부

Supramolecular architectures have lots of potentials in field of organic electronics. Despite of many efforts, simultaneous achievement both in structural aspect and electrical properties was regarded to be very difficult with the only use of self- assembled structure. It is necessary to have functional groups, which are disadvantageous in electrical properties, to build supramolecular architecture. To overcome drawbacks, there has been an increasing study to make hierarchical structures with carbon materials due to its excellent electrical and mechanical properties.Recently, our group reported self-assembled nanostructures, such as nanofiber and nanosheet, by controlling volume fraction of hydrophilic region of amphiphiles.1 These self-assembly molecules are able to disperse graphene and single wall carbon nanotube (SWNT) in aqueous media according to structure analogy. However, the knowledge for intermolecular packing between adsorbent and either carbon materials or themselves was poorly understood. It is necessary to understand supramolecular interaction and their effect on electrical property in order to use carbon material based supramolecular complex into organic electronics. We synthesized two amphiphilic molecules to investigate influence of different hydrophobic region upon supramolecular arrangement on SWNT surface. We demonstrated that alkyl chain moiety within hydrophobic region played an important role in making supramolecular assembly by using structural analysis and molecular dynamics (MD) simulation. We also proved that the ordered supramolecular SWNT-amphiphile complexes show poor electrocatalytic activity due to less effective area to electrolytes. We used two functionalized SWNT as counter electrode, which show 86 %, 68 % as compared to platinum based counter electrodes, with alkyl chain and without alkyl chain respectively.1. Lee, W.; Lee, D. W.; Lee, M.; Hong, J. I., Chem. Commun. 2014, 50, 14851.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-410**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Transition metal catalyzed regio-selective sp3 C-H thioesterification of ether

강병준 홍순혁*

서울대학교 화학부

The first regio-selective thioesterification reaction of ethereal C-H bond has been developed. The reaction is mediated by a dual catalytic system without any stoichiometric oxidant. Since direct transformation of sp3 C-H bond into carboxylic acid derivative has scarcely been reported, we believe that this reaction could open a new platform for step economical carboxylic acid derivative synthesis.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-411**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Application of Carotenoids Molecular Wire

ALAMMOHAMMADSHARIFUL 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carotenoids are fat soluble, colorful pigments serving a variety of rules in cellular biology. They are efficient antioxidants scavenging singlet molecular oxygen and peroxyl radicals. In the human organism, carotenoids are part of the antioxidant defense system. Here, two types of unnatural carotenoids were synthesized. One, carotenoids with anisyl and tolyl substituents at C-13 and C-13' position were synthesized by the coupling of allylic sulfone subunit and dialdehyde subunit. Which were selected for biological study of antioxidation based on the stabilizing of substituent groups. Two, carotenoids containing pyrenylene group at middle position that can be synthesized by the coupling of allylic sulfone and substituted pyrene. These will be investigated for conductance measurement. Ref: 1. Chem. Eur. J. 2013.19, 10832-10835 2. Chem. Eur. J. 2006.16, 7395-7399 3. Org. Biomol. Chem., 2014, 12, 212-232 4. J. Org. Chem. 1999, 64, 6888-6890 5. J. Org. Chem. 1996, 61, 5481-5484

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-412**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study on the Mn(Ⅲ)-initiated radical oxidation and the application on the synthesis of natural products

JIANG XIA 구상호*

명지대학교 화학과

A new type of terpeniod cyclization directed by a β-keto ester moiety has been developed, which proceeded by manganese(Ⅲ)-initiated oxidation of the β-keto ester, followed by an intramolecular hetero Diels-Alder reaction with the terpeniod chain. Based on the mechanism of two steps oxidation, we improved the reaction to be catalytic by the addition of a second cobalt(Ⅱ) oxidant. A high yield was gained under the condition of 5 mol% $Mn(AcO)_3$ and 2 mol% $CoCl_2$. For application, one pot syntheses of furan, thiophene, and pyrrole were accomplished by oxidative deacetylation using Mn(Ⅲ)/Co(Ⅱ) catalysts and the Paal-Knorr reaction from 1,5-dicarbonyl compounds. Further work on extending this catalytic oxidative reaction to the synthesis of some natural products is underway.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-413**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Conversion of Biomass to Pyrrole-2-carbaldehydes:A Sustainable Approach of (-)-Hanishin and Related Natural Products

구상호* **DASADHIKARYNIRMAL**[1]

명지대학교 화학과 [1]명지대학교 에너지융합공학과

Abstract: Readily available carbohydrates (biomass) were converted into N-substituted 5-(hydroxymethyl)pyrrole-2-carbaldehydes (pyrralines) by the reaction with primary amines and oxalic acid in DMSO at 90 °C. Efficient production of pyrrolefused poly-heterocyclic compounds as potential intermediates for drugs, food flavors, and functional materials were achieved by further cyclization of the highly functionalized pyrralines. The mild Maillard variant of carbohydrates and amino esters in heated DMSO with oxalic acid expeditiously produced the pyrrole-2-carbaldehyde skeletons, which were concisely transformed into the pyrrole alkaloid natural products, 2-benzyl- and 2-methylpyrrolo[1,4]oxazin-3-ones and , lobechine , and (−)-hanishin

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-414**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A study on the synthesis of fully conjugated units for lycopene

구상호* 강세인[1]

명지대학교 화학과 [1]명지대학교 에너지융합공학과

Carotenoids are medically and biologically important natural products. We synthesized the natural carotenes by using sulfone-mediated coupling reaction, protection of the resulting alcohol, double elimination of sulfone and protecting alcohol. Recently, lycopene and lycophyll were efficiently produced by using Julia-Kocienski olefination, which can be obtained by the coupling the C10 geranyl benzothiazolyl(BT) sulfone with C20 crocetin dialdehyde. The Julia-Kocienski olefination in the total synthesis of carotenoid natural products were demonstrated using the C5 BT-sulfone containing an acetal group, which was prepared as a chain-extension unit of Apocarotenoids. The double Julia-Kocienski olefination of the C5 BT-sulfone with C10 2,7-dimethyl-2,4,6-octatrienedial and deprotection of the resulting acetal groups efficiently produced C20 crocetin dialdehyde. Above protocol for apocarotenoid can be used the antioxidant activity and electronic conductivity of carotenoids.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-415**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A study of synthetic method for carotene wire

김민수 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Nowadays organic molecular nanowires have been used widely. Nanoscience and engineering requires for the smaller, faster, and flexible substitutes for the conventional metallic wire. Organic molecules containing terminal thiol group can be measured electronic conductance using Atomic Force Microscopy(c-AFM). Carotenoids structure is an ideal organic molecular wire of potentially high electric conductance. Existence of extensive π-conjugation offer high electronic conductance because of the delocalized π-electron system. Organic molecular wires with variable conductance is one of the urgent goals in molecular electronics.We synthesized the carotenoid molecular wires containing terminal thiol group by sulfone-mediated coupling, Ramberg-backlund and double elimination reaction between allylic sulfone and C10-dichloride. We were able to synthesize various morecular wires based on the carotenoid structure and compare the electronic conductance of various molecular wires.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-416**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Study on the Synthesis of fully conjugated chain using chain extension unit

구상호* 김다혜

명지대학교 화학과

Carotenoids are red or yellow pigment in nature, and they are one of the important antioxidant that can prevent cancers. Carotenoids are also used as an element of cosmetics and foods. Since carotenoids cannot be sythesized in human body, they should be supplied from outsides. That is the most important reason that synthesis of carotenoids have been developed in various ways.We previously synthesized the natural carotenes by using sulfone mediated coupling reaction, protection of the resulting alcohol, double elimination. In this research, the synthesis of carotenoids was designed using benzothiazol-2-yl sulfone with crocetin dialdehyde. The Julia-Kocienski olefination enables the efficient preparation of polyenes. So chain extension of isoprenoid using Julia-Kocienski olefination efficiently provided fully conjugated carotenoid compound.The benzothiazol-2-yl sulfone containing an acetal group was prepared as an building block for the chain extension of apocarotenoids. The Julia-Kocienski olefination of the benzothiazol-2-yl sulfone containng an acetal group with 2,7-dimethyl-2,4,6-octatrienedial efficiently produced C20 crocetin dial. The C30 and C40 dials were also prepared from C20 crocetin dial by the repeated application of the Julia-Kocienski olefination of the benzothiazol-2-yl sulfone.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-417**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Research on the synthesis of Unnatural carotenoids

임보람 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Unnatural carotenoids containing various phenyl substituents show excellent characteristics in terms of stability as well as electronic conductance. We have developed a series of efficient synthetic methods of natural carotenoids, which 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. 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 derivatives. The unnatural carotenoids can be synthesized by the coupling/double elimination reaction between allylic sulfone and dialdehyde unit. Therefore, we were able to measure electrical conductivity for the unnatural carotenoid wires.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-418**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation for Tetraphenyl carotenoid wire

정현욱 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Preparation for Tetraphenyl carotenoid wire

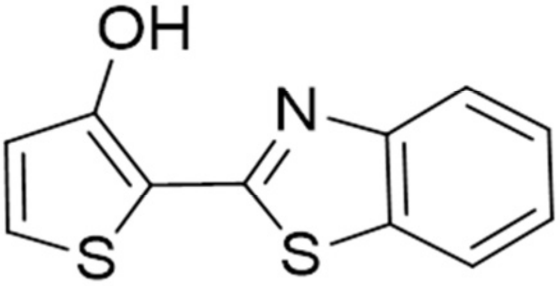
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-419**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

pH Sensitive Fluorescent Probe for Mitochondria Imaging through ESIPT

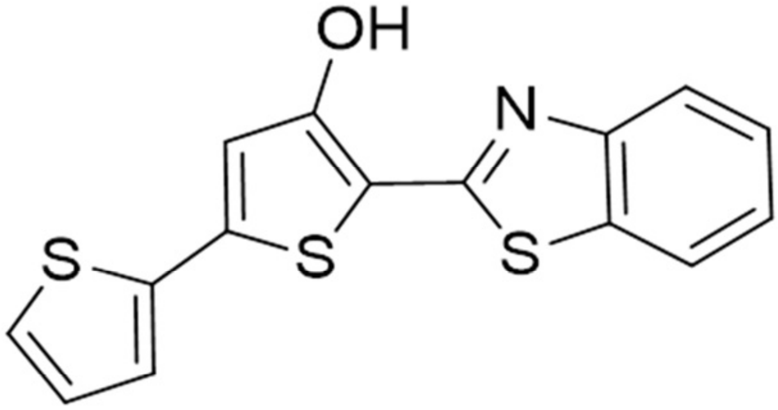
홍경임 장우동*

연세대학교 화학과

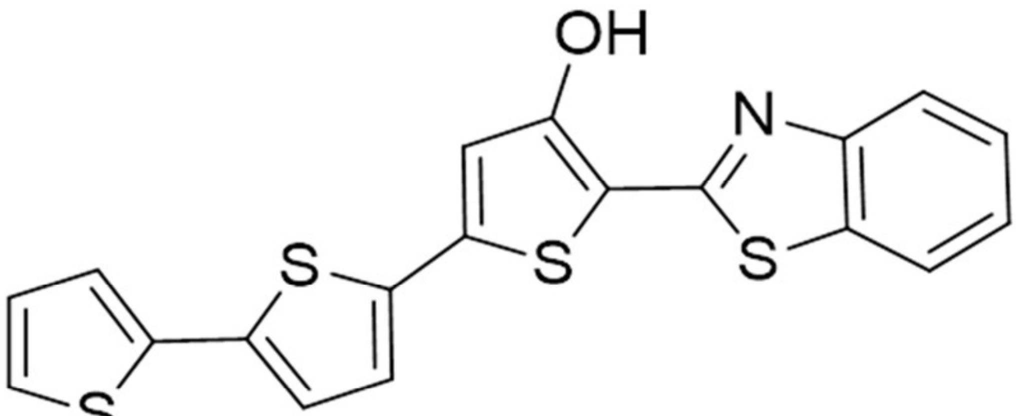
Excited State Intramolecular Proton Transfer (ESIPT) has attracted scientists` attention because it has considerable potential, providing many applications such as molecular probes, luminescent materials, bioimaging probes etc. ESIPT molecules exhibit different fluorescent emissions depending on solvent polarity via phototautomerization. The most remarkable property of ESIPT is a large stokes shift which prevents self-absorption problem of fluorescence emission. We have synthesized a series of thiophene-based ESIPT molecules, that are oligothiophene conjugated with benzothiazole group (**nT-HBT**; n = 1, 2, and 3, n is number of thiophene units). **2T-HBT** clearly exhibited dual emissions according to solvent polarity; green emission in non-polar solvent and blue emission in aprotic solvent. Interestingly, **2T-HBT** showed clear emission enhancement at small pH value change (at pH 7~8). This effective turn-on process at the narrow pH range can be utilized as effective bio probes. Upon in vitro evaluation, **2T-HBT** exhibited selective staining of mitochondrial compartment. We are going to report detailed aspect of the thiophene-based ESIPT probes.



1T-HBT



2T-HBT




사단법인 대한화학회
KOREAN CHEMICAL SOCIETY

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-420**

발표분야: 유기화학

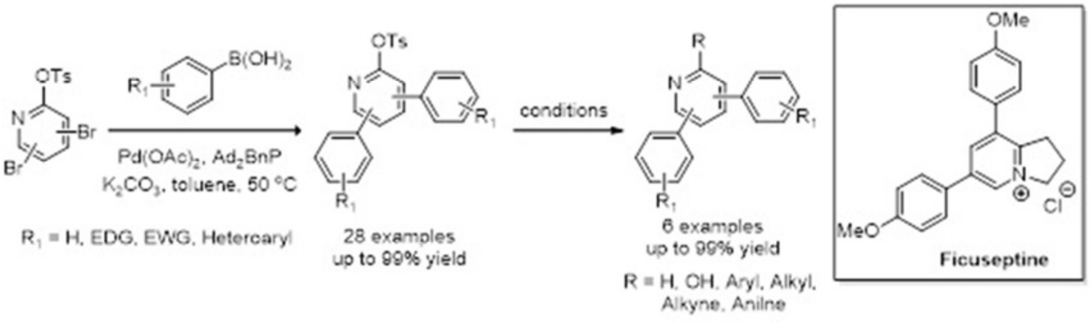
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Trisubstituted Pyridines via Chemoselective Suzuki-Miyaura Coupling of 3,5- and 4,6-Dibromo-2-tosyloxypyridines

박초희 권용주[1] 김원석*

이화여자대학교 화학 나노과학과 [1]이화여자대학교 화학나노과학과

Heterocycles including pyridine are one of the most widely studied classes. Pyridine and its derivatives are easily found in natural products and of great importance in synthetic chemistry, pharmaceutical and agrochemical research. Therefore, numerous synthetic methods have been reported to form functionalized pyridines. Palladium catalyzed cross coupling reaction is one of the most convenient and versatile method for the preparation of trisubstituted pyridines from polyhalogenated pyridines. Therefore, regioselective Suzuki-Miyaura reactions on 3,5- and 4,6-dibromo-2-tosyloxypyridine have been studied. Herein, we reports the optimized conditions allow for facile access to 3,5- and 4,6-diaryl-2-tosyloxypyridines in yields of 8 to 99%. Further functionalization of the tosylate group in the diarylpyridine derivatives obtained was accomplished for the synthesis of novel and biologically relevant trisubstituted pyridines. The formal synthesis of ficuseptine, a bioactive alkaloid, also has been achieved via palladium-catalyzed cross-coupling reaction of 3,5-dibromo-2-tosyloxypyridine in 5 steps with 48% overall yield from 3,5-dibromo-2-hydroxypyridine.



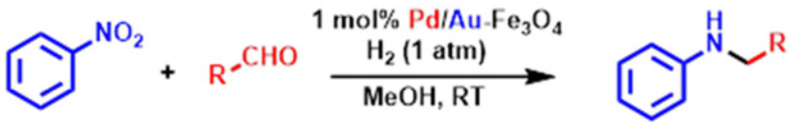
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-421**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

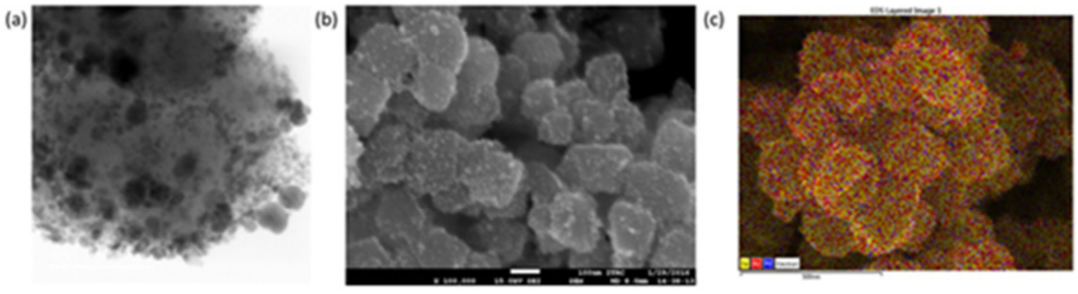
Synthesis of bimetallic Pd/Au-Fe_3O_4 and their application as magnetically recyclable catalysts for reductive amination

조아라 변상문 김병문*

서울대학교 화학부

Recently, we have reported several simple catalytic reactions based upon Pd–Fe_3O_4 heterodimeric nanocrystals as magnetically reusable catalysts. Successful applications of the nanocrystals toward various organic reactions. To improve limitations of monometallic reaction systems including catalyst deactivation and requirement of base in some metal-catalyzed reactions, a bimetallic system is considered. Bimetallic systems can often overcome many drawbacks, combining the properties involved in the two individual metals. The synergistic effect of bimetallic system has been reported for different applications. Hereupon we report on the preparation of Pd/AuFe_3O_4 bimetallic nanoparticles by simple and fast synthetic route and the application of the nanoparticles toward practical synthesis of mono N-alkyl amines using tandem reduction of nitroarenes and reductive amination with aldehydes. Thus, the new catalyst system could offer a very sustainable, environment-friendly tool useful for potential industrial applications in the reductive amination reaction of nitro compounds





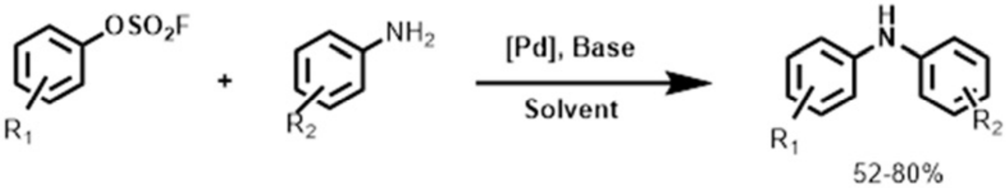
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-422**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Palladium-catalyzed, ligand-free amination of aryl fluorosulfonates

임태현 김병문*

서울대학교 화학부

Diaryl amines are becoming ever more useful intermediates in many applications such as drugs, photoelectric materials, etc. Amination of aryl halides with aryl amines have been reported employing palladium catalysts with an array of ligands. We report herein direct amination of aryl fluorosulfonates with aryl amines using a palladium catalyst. This cross coupling reaction occurs under mild conditions with a tetrakis(triphenylphosphine)palladium(0) without any use of a special ligand or additional additives, which are essential for the previously reported aminations. Aryl fluorosulfonates can be prepared in quantitative yields from the reaction of phenol derivatives and sulfuryl fluoride, and offer readily available coupling partners for the amination reactions as alternatives to aryl halides or other aryl sulfonates.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-423**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Catalytic Asymmetric Construction of α-Silyl Ketone Using Diazo Compounds and Aldehydes

김재연 강기태 신성호 **JINHUI** 심수용 김태형 남동국 김승태 조수민 류도현*

성균관대학교 화학과

α-Silyl ketones are useful building blocks in organic synthesis because they are substrates for many regio- and stereoselective reactions to construct carbon-carbon and carbon-heteroatom bonds in high stereoselectivities. Despite a growing focus toward synthetic efforts, access to chiral silanes in a highly enantioenriched form remains a great challenge and the development of new methods continues to be an active area of research. In this research, we developed highly enantioselective method for the synthesis of α-silyl ketones catalyzed by chiral boron catalyst. The synthetic utility of this method was demonstrated by the synthesis of chiral 1,2-diols.1. Sun, C.; Li, J.; Demerzhan, S.; Lee, D. ARKIVOC 2011 (IV) 172. Chen, D.; Zhu, D.; Xu M. J. Am. Chem. Soc. 2016, 138, 1498.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-424**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A convenient synthesis of tropane ring structure via an oxidative Mannich-type cyclization

조한별 Ahmed H. E. Hassan[1] 이재균[2] 조용서[3,*] 민선준[4,*]

한양대학교 응용화학과 [1]과학기술연합대학원대학교(UST) 화학과 [2]한국과학기술연구원(KIST) 케모인포매틱스연구단 [3]한국과학기술연구원(KIST) 생체과학연구본부 [4]한양대학교 과학기술대학/응용화학과

Tropane alkaloids are a group of alkaloids generally derived from natural plants and they contain a unique azabicyclic[3.2.1]octane ring structure. They are often found as secondary metabolites in many members of the plant families such as Erythroxylaceae and Solanaceae. The alkaloid analogues which include tropane structure have been manufactured as active pharmaceutical ingredients (APIs) for a long time. In particular, several tropane derivatives can regulate biological receptors associated with neurotransmission, which may be useful for the treatment of neurological or psychological disorders. Therefore, the tropane alkaloids are highly attractive targets to organic chemists due to their pharmacological importance as well as structural complexity.In this study, our synthetic approaches towards tropane alkaloids via oxidative Mannich cyclization were described. Our synthetic plan includes oxidative coupling reaction of cyclic amine with acetone followed by intramolecular Mannich-type cyclization to afford tropane core structure. In this event, direct C-H activation of cyclic amine by an oxidant to generate the corresponding iminium intermediate is a crucial transformation for consecutive C-C bond formations, which will be focused on in this presentation. In addition, development of a chemical library of tropane derivatives will be further discussed.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-425**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Comparison of Column Separation Conditions of Some Anhydride-Imides and Diimides Synthesized from Dianhydrides and Amines

김성식

전북대학교 화학과

Several anhydride-imides and diimides were prepared to investigate their spectroscopic and photophysical properties using laser flash photolysis and other spectroscopic techniques. Double carboxylic acid anhydride such as pyromellitic dianhydride and naphthalene tetracarboxylic dianhydride were used as the starting materials for the synthesis of the target molecules. Column separation conditions of the anhydride-imide and diimides were compared based on the eluents. The imides studied here include anhydride-imides containing benzene and naphthalene ring, diimide containing benzene and naphthalene moiety, and two diimides connected by phenyl ring.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-426**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Stereoselective Synthesis of 6-Alkylidene/Benzylidene-Isoindolo[2,1-*a*]indoles through Pd-catalyzed 5-*exo-dig* cycloisomerization

ALAM KHYARUL 박진규*

부산대학교 화학과

Cycloisomerization reactions are versatile and atom-economical strategy to generate cyclic organic compounds from acyclic starting materials. For the synthesis of N-heterocyclic compounds which are highly important class of compounds found in various natural products, biologically active structures and medicinally relevant compounds, utilization of ynamides has expanded enormously.[1] Isoindolo[2,1-*a*]indole is one of functionalized indoles that have been synthesized by employing classical synthetic organic, photochemical, radical and palladium-mediated methodologies.[2] However, no reports containing alkylidene/benzylidene moieties at C-6 of the isoindolo[2,1-*a*]indole structure have appeared.Herein, we described Pd-catalyzed synthesis of 6-alkylidene/benzylidene-isoindolo[2,1-*a*]indole, which was accomplished via steroselective 5-*exo-dig* cycloisomerization of ortho aryl palladium species generated through C-H activation. Also, this 6-alkylidene/benzylidene-isoindolo[2,1-*a*]indoles can be utilized as synthetic precursor for the synthesis of highly functionalized and biologically important isoindolo[2,1-*a*]indoles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-427**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Base-Controlled Cu-Catalyzed Tandem Cyclization and Alkynylation for the Synthesis of Indoles and Indolizines

오경환 김성민 박선영 박진균*

부산대학교 화학과

Over the last decade, transition metal-catalyzed aminometallation[1] of alkynes has been widely used for the synthesis of heterocycles such as indoles and indolizines. A tandem reaction strategy has been used to access diversely functionalized N-heterocycles as well; utilizing a metal-bound intermediate generated in situ for the subsequent C-C coupling reaction with pre-chosen reagents.[2,3] The procedure benefits from good atom and step economy, offers flexibility in constructing the organic backbone, and has excellent selectivity in C-C bond forming reaction. To date, while a few example of Rh and Pt catalysis are known for tandem addition reactions in the indole synthesis, most examples are limited to Pd catalysis for the synthesis of indoles and indolizines involving cycloisomerization, followed by C-C coupling reactions. These methods, however, require harsh reaction conditions and expensive metal and ligand. Interestingly, copper-catalyzed tandem C-C coupling reaction has rarely been explored despite of copper metal's natural abundance and cheap price. Recently, we have developed a base-controlled Cu-catalyzed tandem cyclization/alkynylation of propargylic amines, which provides rapid access to functionalized indole and indolizine[4] derivatives under mild reaction conditions. The reaction first proceeded via a 5-*endo-dig* aminocupration, followed by a coupling between the copper-bound intermediate and alkynyl bromide, to afford the products in good to excellent yields. The successful tandem reaction for excellent selectivity is attributed to the unique property of the bases, DBU (1,8-diazabicyclo[5.4.0]undec-7-ene) and MTBD (7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-428**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Copper-Catalyzed N-Arylation of 2-Pyridones Employing Diaryliodonium Salts at Room Temperature

정서희 김원석*

이화여자대학교 화학 나노과학과

N-aryl heterocycles have attracted synthetic organic chemists due to their intriguing biological activities. In particular, N-aryl pyridine-2(1H)-one is an important moiety present in biological active compounds such as Pirfenidone, Perampanel and Amphenidone. Therefore, numerous synthetic methods have been reported to form C-N bond between 2-pyridones and either aryl halides or aryl boronic acids as a coupling partner. Herein, a mild and efficient method for the synthesis of N-aryl pyridine-2(1H)-one is demonstrated by using various diaryliodonium salts as an electrophilic coupling partner at room temperature. Most reactions proceed readily at room temperature in the presence of 10 mol% of copper chloride. As a result, a wide range of N-aryl pyridine-2-ones were synthesized in yields of 23% to 99%. We have also investigated the synthesis of Pirfenidone which was successfully synthesized in 99% yield within 30 min at room temperature.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-429**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

L-Proline catalyzed enantioselective synthesis of β-carbonyl amino acid derivatives via *anti*-Mannich reaction of cyclicimines with ketones

김동환 이희순[1] 정재경[1,*]

충북대학교 약학대학 [1]충북대학교 제약학과

β-carbonyl amino acid derivatives represent an important structural unit have always fascinated by organic chemists because of its ubiquitous in nature, found in many natural and bioactive compounds. Over the years, number of approaches have been developed, among them Mannich reactions are very well known method. Considerable efforts have been devoted toward the development of *syn*-Mannich reaction. On the other hand, there are only few reports are available for the synthesis of *anti*-Mannich product, though most of the approaches were using β-proline and other and costly catalysts. Thus far, the development of efficient approach for *anti*-Mannich reaction by using economically cheap catalyst is in high demand. In this study, we have developed highly enantioselective *anti*-Mannich reaction of various cyclicimines with ketones by using simple L-proline (30 mol%) as catalyst. When unsymmetrical ketone used as Mannich donor, we have obtained linear product as major over the branch. The protecting group can be easily removed and furnished α-amino acid derivatives. By using our optimized condition, wide range of β-carbonyl amino acid derivatives were directly obtained in shorter reaction time in *anti*-conformation with excellent enantiomeric excess (up to 99% ee) and diastereoselectivities (dr ratio, up to 10:1).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-430**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enantioselective Aza-Michael Addition of Amide: Application to Synthesis of Piperidone derivatives

이정태 조혜주 이희순[1] 정재경[1,*]

충북대학교 약학대학 [1]충북대학교 제약학과

The aza-Michael addition is the conjugate amination of α, β-unsaturated carbonyl compounds and it is one of the useful reaction for formation of C-N bond. Typically, the asymmetric aza-Michael addition catalyzed by chiral imidazolidinone or pyrrolidine has been reported in the literature where it proceeds via the iminium ion activation of α, β-unsaturated carbonyl compounds by chiral secondary amines, thereby facilitating the addition of the nitrogen nucleophiles. However, these nucleophiles have been limited to carbamates, imides, pyrroles, pyrazoles and triazoles.As far as we know, this is the first report of an enantioselective organocatalytic aza-Michael addition of amides as nitrogen nucleophiles. Furthermore, this reaction is applicable to synthesis of piperidone derivatives.

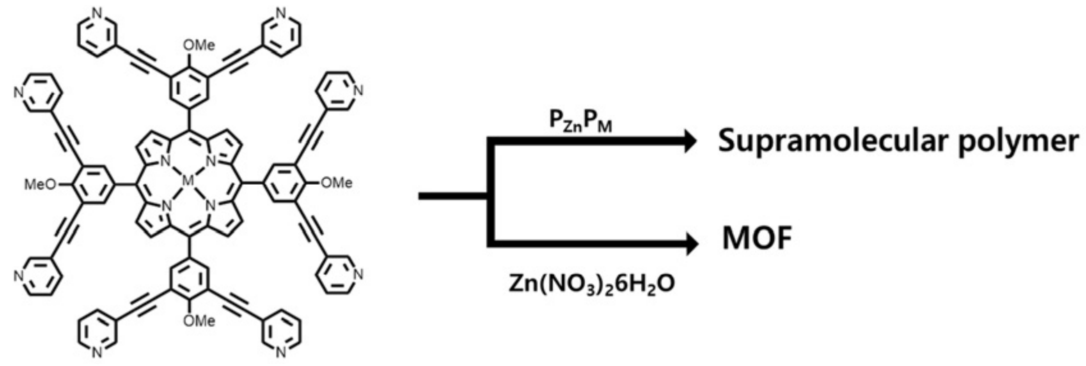
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-431**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Multipyridyl Porphyrin for Supramolecular Coordination Polymer

이호수위 장우동*

연세대학교 화학과

We newly design an organic building block, multipyridyl-bearing porphyrin $\mathrm{PyP_M}$ ($\mathrm{M=H_2}$ or Cu), composed of peripheral 8 pyridyl groups attached to focal freebase or copper porphyrin thorough acetylene bridge. We previously reported an artificial light-harvesting dendrimer $\mathrm{P_{Zn}P_{FB}}$, 8 zinc porphyrin wings ($\mathrm{P_{Zn}}$) attached to the focal freebase porphyrin ($\mathrm{P_{FB}}$), that exhibits efficient energy transfer from the $\mathrm{P_{Zn}}$ wings to the core $\mathrm{P_{FB}}$. As $\mathrm{PyP_M}$ were added to the dendrimer, supramolecular polymer was formed through multiple axial coordination interaction between pyridyl groups of $\mathrm{PyP_M}$ and $\mathrm{P_{Zn}}$ wings in $\mathrm{P_{Zn}P_M}$. UV/Vis absorption spectra were recorded upon titration of $\mathrm{PyP_{FB}}$ to $\mathrm{P_{Zn}P_{FB}}$. Differential spectra was obtained and exhibited clear isosbestic points with saturation binding at 1 equivalent addition of $\mathrm{PyP_{FB}}$ to $\mathrm{P_{Zn}P_{FB}}$. Job's plot analysis also indicated 1:1 stoichiometry for the saturation binding. The fibrous assembly of $\mathrm{P_{Zn}P_{FB}}$ and $\mathrm{PyP_{FB}}$ was well visualized by atomic force microscopy (AFM) and transmission electron microscopy (TEM). The fluorescence emission measurement of $\mathrm{P_{Zn}P_M}$ indicated efficient intramolecular energy transfer from $\mathrm{P_{Zn}}$ of $\mathrm{P_{Zn}P_M}$ to the focal $\mathrm{P_{FB}}$ or $\mathrm{P_{Cu}}$ of $\mathrm{PyP_M}$. As the structural rigidity of $\mathrm{PyP_M}$, PyP-MOF(Zn) were prepared using $\mathrm{PyP_M}$ as a ligand. To obtain visual evidence of PyP-MOF(Zn), we examined the MOF through the scanning electron microscopy(SEM) and SEM images show amorphous 2-dimensinal sheets.



PyP_M
($M=H_2$ or Cu)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-432**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A new class of tripodal glucose-cored amphiphiles (TGAs) for membrane protein study

EHSANMUHAMMAD 채필석[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 생명나노공학과

Most membrane proteins exist in complexes with other proteins rather than isolated entities. To fully understand their biological functions it is essential to study the intact membrane protein assemblies. The overexpression and purification of many membrane protein complexes is still a considerable and unsurmountable challenge. In the case of membrane protein complex, thus, protein extraction from a source as a large multi-subunit cellular complex is necessary for the structural analysis. Detergents are indispensable tools in the isolation of membrane protein complexes from the biological membranes for downstream characterization. Here, we designed a glucose-cored family of detergents containing tripodal hydrophobic group. These novel agents were evaluated for a set of membrane proteins including a G-protein coupled receptor (GPCR). Among all of them, TGA-E8 displayed favorable behaviors for all targeted membrane proteins, indicating that this TGA has a significant potential in membrane protein structural study.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-433**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and evaluation of trialkylated glucoside amphiphiles for membrane protein study

GHANI LUBNA 채필석[1,*]

한양대학교 bio nano engineering [1]한양대학교 생명나노공학과

Membrane proteins are crucial components for a number of cellular functions, but are difficult to study their structure and functions because these bio-macromolecules are generally unstable when removed from their native membranes. A number of new detergents, lipids and non-detergent-like amphiphiles have been developed to stabilize membrane proteins, and these membrane-mimetic systems have contributed to successful determinations of membrane protein structures in recent years. Despite these successes, however, currently available reagents are inadequate and there remains a pressing need for new amphiphiles with unique structural features. To this end, we synthesized trialkylated glucoside amphiphiles with a new type hydrophilic group. When these highly branched glucoses were evaluated for UapA and LeuT stability, we found that some of new agents displayed favorable properties toward the targeted membrane protein, indicating potential use of these agents for membrane protein study.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-434**

발표분야: 유기화학

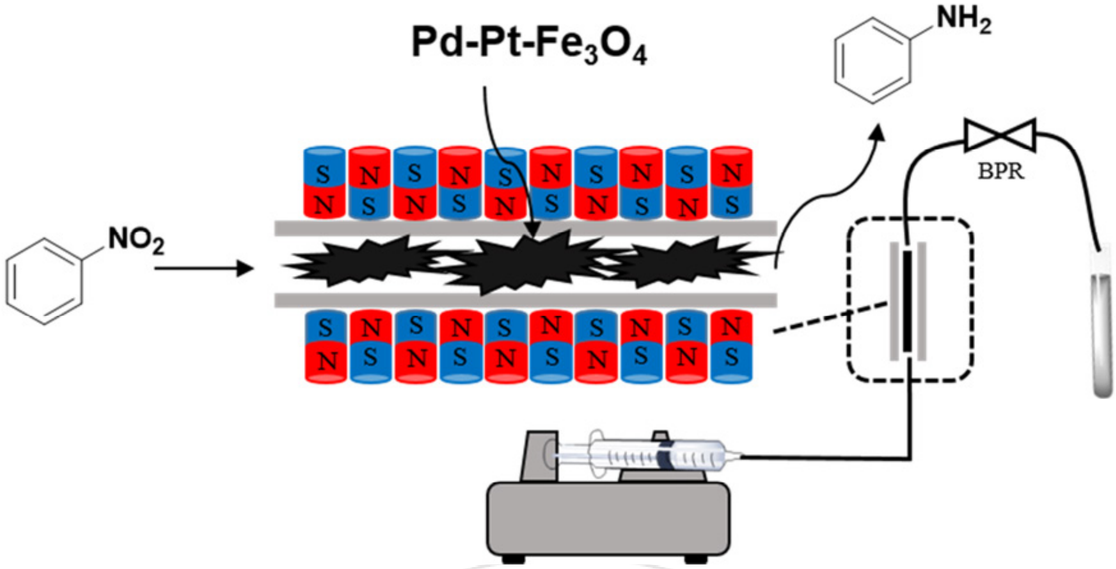
발표종류: 포스터, 발표일시: 금 11:00~12:30

Continuous-Flow Hydrogenation of Nitroarenes Using Magnetic Pd-Pt-Fe_3O_4 Nanoflakes

김홍원 김성민 박진균*

부산대학교 화학과

Continuous-flow reaction technique for organic synthesis has many advantages when compared to batch reaction. Safer reactions could be ensured when handling hazardous chemicals because the flow reaction of small amounts of materials enables easy mixing and heat control. Furthermore, gas evolution with high pressure could be easily controlled by a back pressure regulator (BPR). Therefore, flow reaction technique has already been demonstrated that fine chemicals, such as natural products or active pharmaceutical ingredients could be scaled up in academia as well as in pharmaceutical industry. One of the types of continuous flow systems is immobilizing catalyst in the continuous reactor which we are interested in. Recently, Kim et al. has reported the preparation of magnetic bimetallic Pd-Pt-Fe_3O_4 NPs, which exhibited as efficient heterogeneous catalyst for the reduction of nitroarene using ammonia-borane as reducing agent at room temperature. Magnetic bimetallic catalyst was easily recycled more than 200 times using an external magnet, however, we thought that it would be more beneficial if the catalyst could be applied in flow for the continuous production of the desired product. Also, we considered ammonia-borane a very practical reagent for the continuous reaction because of its high stability and good solubility in organic solvent. Finally, we have demonstrated the easy reversible fixation of Pd-Pt-Fe_3O_4 nanoflakes in tubing using neodymium magnet and reduced nitroarenes to anilines using ammonia borane. Under the optimized continuous-flow hydrogenation protocols, a variety of nitroarenes were tolerated with excellent yields.


Pd-Pt-Fe$_3$O$_4$
NO$_2$
NH$_2$
BPR
S N S N S N S N S N
N S N S N S N S N S

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-435**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Tandem neopentyl glycol-based maltosides with a short linker for analysis of membrane proteins

배형은 채필석[1,*]

한양대학교 바이오나노학과 [1]한양대학교 생명나노공학과

Membrane proteins are main players for many cellular functions. Research on membrane proteins has brought significant attention in scientific community. However, membrane protein research is tremendously difficult mainly due to their inherent amphipathic characteristic. Accordingly, many membrane proteins have strong tendency to aggregate and denature in an aqueous solution. Amphipathic molecules called detergents are widely used as essential tools to solve the issues associated with membrane protein analyses. However, conventional detergents often have serious limitation at maintaining protein activity in a sufficiently long term for protein structural determination. In the present study, we synthesized four tandem neopentyl glycol-based maltosides with a short linker, designated TNM-Ss, and characterized their micellar properties. When evaluated with a few membrane proteins, these agents displayed favorable behaviors compared to conventional detergents for the proteins targeted here.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-436**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Palladium-Catalyzed Direct Arylation of [1,2,4]triazolo[1,5-*a*]pyridines at the C5 and C8 position

박선영 박진규*

부산대학교 화학과

[1,2,4]Triazolo[1,5-*a*]pyridines are one of the typical kinds of fused N-heterocyclic compounds. They have frequently been used in pharmaceuticals, herbicides, fluorescent brighteners, electronic materials.[1,2] Especially, C5 substituted [1,2,4]triazolo[1,5-*a*]pyridines are important structural motif such as DNA-dependent protein kinase, stabilizing agents for photographic emulsions, antibacterial agents, selective adenosine receptor antagonists and several inhibitors, such as PDE inhibitors, selective JAK1 inhibitors, and TGFβ receptor inhibitors.[3] And C8 substituted [1,2,4]triazolo[1,5-*a*]pyridines are utilized for electronic devices. Despite their clear importance, installation of an aryl group at the C5 and C8 positions of triazolopyridine still remains a challenge and only achieved via conventional multi-step process.[4] From the perspective of atom and step economy, the development of direct arylation would be attractive for rapid and systematic generation of useful heterocycles. Herein, we will present a new method for direct syntheses of C-5 and C-8 substituted [1,2,4]triazolo[1,5-*a*]pyridines using a Pd catalyst.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-437**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Vicinal Chlorotrifluoromethylation with photorededox catalysis

한홍식 이영진[1] 이현명[2] 김균은[3] 김재학[4] 정영식[5] 한수봉[6,*]

과학기술연합대학원대학교(UST) 의약화학(한국화학연구원) [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 난치성질환치료제연구그룹 [3]과학기술연합대학원대학교(UST) 한국화학연구원/의약화학및약리생물학과 [4]한국화학연구원 난치성질환치료제연구센터 [5]한국화학연구원 신물질연구단 [6]한국화학연구원 신약연구본부

ABSTRACT 1,2-Difunctionalization of alkynes is one of the simple and efficient method for synthesis of complicated and multi-functionalized molecules. Herein, a method for Chlorotrifluoromethylation of internal alkynes to form substituted olefins via visible light-promoted photoredox catalysis was developed. High regio- and stereoselectivity was observed during the incorporation of trifluoromethyl and chloride moiety. The reagent CF_3SO_2Cl is used as both CF_3 radical and chloride ion source in the presence of $Ir(ppy)_3$ catalyst. The trifluoromethyl substituted vinyl chloride products can be further transformed to more valuable compounds.

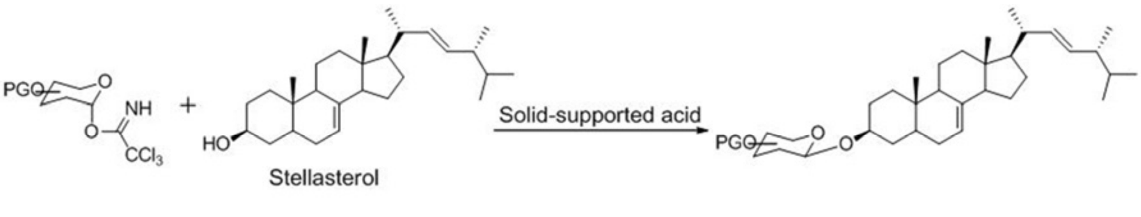
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-438**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly efficient green glycosylation of stellasterol promoted by solid-supported acid

오현정 조영경[1] 박훈규 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Natural spinasterol-glucose (3-O-β-D-glucopyranosylspinasterol) has been identified as a compound to exhibit strong anti-inflammatory activity. However, spinasterol-glucose is difficult to isolate from natural plants or synthesize. To overcome these difficulties, we have already designed and synthesized β-glucosyl stellasterol by Lewis acid-catalyzed glycosylation of trichloacetimidates with a sterol. However, this synthetic procedure seems to be not good in a large scale production due to a slightly low yield and the use of highly moisture sensitive Lewis acid. Therefore, we have used a solid-supported acid catalyst instead of Lewis acid. Solid-supported acid catalysts have several advantages over liquid acids such as no work-up, easy separation, and easy recovery and reusability. In this report, we suggest the highly efficient green process for the glycosylation using solid-supported acid-catalyst to yield several glycosyl stellasterols in high yields.



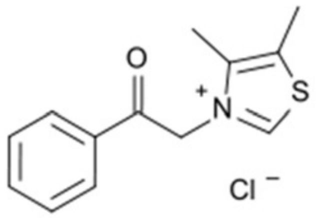
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-439**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of 1,4-naphthoquinone Derivatives and Potential Activity for AGE

박슬찬 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

1,4-Naphthoquinones have recently emerged as a potent antitumor, anti-virus, anti-parasitic, and anti-inflammatory agent in vitro, and in vivo. Advanced glycation end-products(AGEs) are proteins or lipids that become glycated as a result of exposure of sugars. They can be a factor in aging and in the development or worsening of many degenerative diseases, such as diabetes, atherosclerosis, chronic renal failure, and Alzheimer's diseases. In this work, we have synthesized 1,4-naphthoquinone derivatives and tested for the AGE breaking potential, which would be used for the treatment of aging and age-related diseases. Alagebrium is a compound that is thought to break some existing AGE crosslinks.



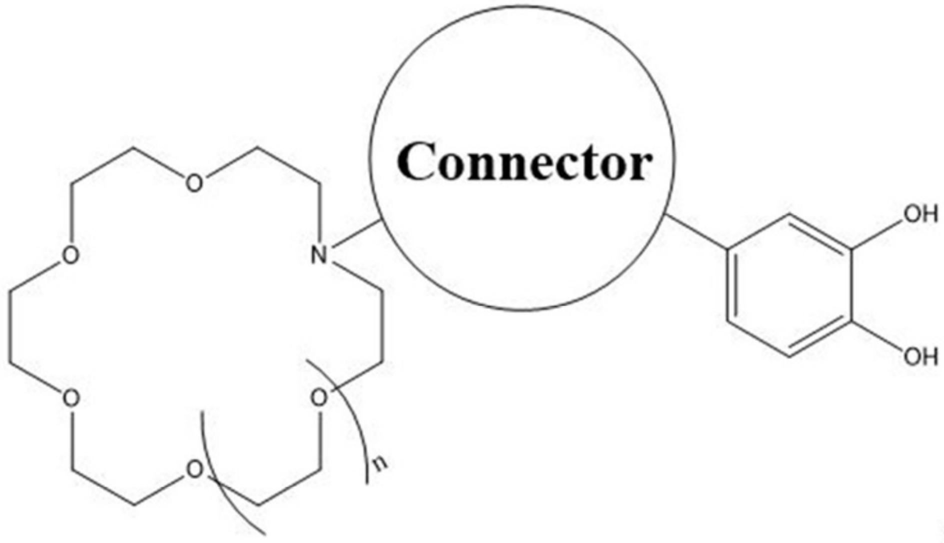
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-440**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Catechol-containing Azacrown Ethers for the Metal Extraction in Supercritical CO_2

김유로 **yan xinhao** 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Catechol and azacrown ether derivatives have been used for the metal extraction through a special metal binding. In this work, we have synthesized several catechol-containing azacrown ethers to show a high CO_2-solubility and tested for the metal extraction in supercritical carbon dioxide ($scCO_2$). The relationship between structure and CO_2-solubility, and structure and extractability have been studied.



일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ORGN.P-441**

발표분야: 유기화학

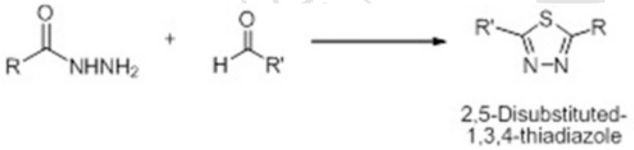
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Highly Efficient One-pot Synthesis of 2,5-Disubstituted-1,3,4-Thiadiazoles from aldehyde and hydrazide Using Lawesson's Reagent

<u>박수진</u> 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

1,3,4-Thiadiazole derivatives are the most common and well-known heterocyclic compounds due to their broad bio-active spectrum such as antituberculosis, antioxidant, anti-inflammatory, anticonvulsants, antidepressant, anxiolytic and antihypertensive.In this study, we prepared 2,5-disubstituted-1,3,4-thiadiazole derivatives from a hydrazide and an aldehyde in one-pot reaction. A reaction of aldehyde with hydrazide gives *N*-acylhydrazone, followed by reacting with Lawesson's reagent in the presence of amine base to afford a 2,5-disubstituted-1,3,4-thiadiazole in a high yield.



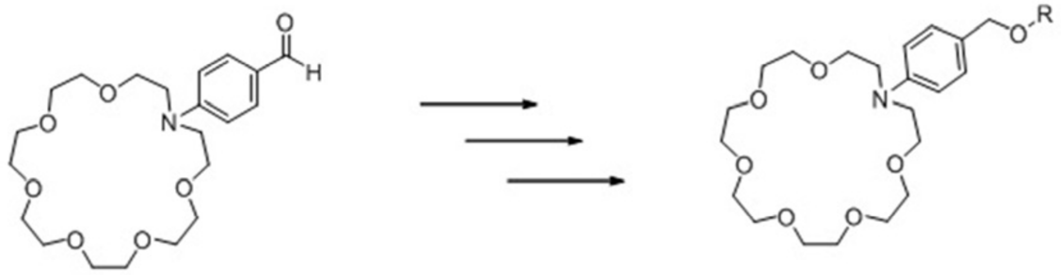
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-442**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and evaluation of new aza-21-crown-7-ether derivatives as a CO2-soluble chelating agent

송희 박예슬[1] 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

In present study, new CO2-soluble aza-21-crown-7-ether derivatives have been designed and synthesized from N-(4-formylphenyl) aza-21-crown-7-ether by simple chemical modifications for the development of a CO2-philic chelating agent. Their CO2-solubilities and metal extraction ability in supercritical carbon dioxide (scCO2) have been tested and the relationship between structure and CO2-solubility, and structure and extractability have been studied.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-443**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Intramolecular Fischer indole synthesis for the direct synthesis of 3,4-fused tricyclic indole and application to the total synthesis of (-)-aurantioclavine

박준 <u>김동현</u> **DAS TAPAS** 조천규*

한양대학교 화학과

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

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-444**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

New concise total synthesis ningalin D

김장엽 김동현 조천규*

한양대학교 화학과

Naphthalene is an important structural subunit frequently found in natural products, pharmaceuticals, and everyday-life products. By using 2-pyrone derivatives and benzyne as a diene and dienophile in Diels-Alder reaction, we prepared various poly-substituted naphthalenes in excellent yield. In conjunction to our ongoing study on aryl hydrazides, we have elaborated a new synthetic route to ningalin D by way of dibenzo-carbazole **6** readily accessible by the [3,3]-sigmatropic rearrangement of dinaphthyl hydrazide **5** and cyclization of the resulting diamine product. Introduction of two 3,4-dimethoxyphenyl groups and oxidations would culminated in the synthesis of ningalin D. Presented herein will be our recent efforts in the synthesis of poly-substituted naphthalenes and application to the synthesis of ningalin D.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-445**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Asymmetric total syntheses of (+)-aspidospermidine and (-)-tabersonine via regio-controlled Fischer indole synthesis

조현규 김주영 조천규*

한양대학교 화학과

Recently we have demonstrated that ene-hydrazide readily available from enol triflate in regiochemically defined form may undergo Fischer indolization reaction with no regiochemical scrambling. In order to prove its usefulness, we then started to apply our new method to the syntheses of various aspidosperma alkaloids. The aspidosperma family comprises the largest group of indole alkaloids, with more than 250 compounds. The structural challenge posed by these alkaloids in conjunction with the potent pharmacological properties exhibited by several members has stimulated considerable effort directed toward their synthesis. Prior to syntheses of a variety of intricate aspidosperma alkaloids, we initiated synthesis of (+)-aspidospermidine, the simplest aspidosperma alkaloid. With carbamate **1** in hand, the carbamic anion mediated Michael addition followed by triflation gave us bicyclic compound **2** in high yield. Subsequent regioselective Fischer indolization under Lewis acidic conditions culminated in the synthesis of (+)-aspidospermidine **3**. It substantiated that our strategy is indeed quite efficient in the syntheses of aspidosperma alkaloids. Based on the initial success, we are investigating the syntheses of other more complicated aspidosperma alkaloids. Presented herein are the total synthesis of (+)-aspidospermidine and our recent progress toward (-)-tabersonine.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-446**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Progress toward total synthesis of (±)-clivonine

WANGCHENGDONG 조천규*

한양대학교 화학과

Diels-Alder reaction of 2-pyrone can be exceptionally powerful for the synthesis of structurally complex natural products, constructing multiple carbon-carbon bonds in a single operation. As a part of our ongoing study exploring the utility of 3,5-dibromo-2-pyrone in target-oriented synthesis, by using the highly endo-selective, we have further envisioned that the same synthetic strategy should be effective for Clivonine that using(E)-β-borylstyrene as a dienophile for the key Diels-Alder reaction with 3,5-dibromo-2-pyrone.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ORGN.P-447**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

New concise total syntheses of (-)-neocosmosin A and ent-(-)-monocillin IV via Intramolecular Diels-Alder reaction of 2-pyrone

이준호 조천규*

한양대학교 화학과

Resorcyclic acid lactones (RALs) are polyketide-derived benzannulated macrolides, named for their resorcyclate core structure fused to a 12- or 14-membered lactone ring. Many of them exhibit intriguing biological activities that include anticarcinogenic, antimalarial, antifungal, and antibiotic properties. Several RAL compounds are in fact currently under development for the clinical applications. Because of their potential values as new drug candidates, invention of methods and/or routes that allow rapid and divergent synthesis of RALs would be of significant interest. Neocosmosin A is a recently found RAL, co-isolated with neocosmosin B and C from a fungus *Neocosmospora* sp. (UM-031509) in 2012. It was shown to have a strong binding affinity for human opioid and cannabinoid receptors.

As a part of our ongoing study on 3,5-dibromo-2-pyrone toward target oriented synthesis, we have devised A new synthetic route to (-)-neocosmosin A and ent-(-)-monocillin IV were devised through the elaboration of intramolecular Diels-Alder cycloaddition of 2-pyrone containing bromo-propiolate group as dienophile. The IMDA reaction was accompanied with cycloreversion of carbon dioxide to give benzannulated macrolide with two bromide groups at C14 and C16. Installation of the pinacolboryl groups and oxidations allowed the total syntheses of neocosmosin A and ent-monocillin IV.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-452**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Well-Defined Polymer-Photosensitizer Complex Obtained by "Click-Chemistry" Method for Enhanced Photodynamic Therapy

LIU YANG 윤일[1,*]

인제대학교 school of nanoscienc [1]인제대학교 PDT 연구소

Well-defined polymer(WDP)-photosensitizer(PS) complex was prepared by using azide-photosensitizer and alkynyl-polymer with "Click Chemistry" method.The WDP-PS complex is a promising agent for enhenced photodynamic therapy with distrinctive properties and functions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-453**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design, Synthesis, and Antiproliferative Activities of Novel Arylamino(indazol-3-yl)urea Derivatives against Bladder Cancer Cell Line

최성은 최민정 김종승 유경호[1,*]

고려대학교 화학과 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

Bladder cancer represents the fifth most common neoplasms in developed countries and a major cause of cancer-related morbidity and death. Incidence and mortality rates have remained relatively constant over the past four decades, with an estimated 72,570 new cases and 15,210 deaths predicted for 2013 in the United States alone. Their conventional treatment involves surgical resection and intravesical chemo- or immunotherapy. Despite advances in the surgical and medical treatment, there have only been limited improvements in disease-specific mortality rates over the past decades. Epithelial cancers such as bladder cancer also exhibit deregulation and mutation of FGFR3, but whether this contributes to tumorigenesis in vivo has remained unclear.The purpose of this study is to develop the potent compounds for the treatment of bladder cancer. A series of arylamino(indazol-3-yl)urea derivatives with a novel hinge moiety, based on the structural features of AZD4547, were designed and synthesized. And their in vitro antiproliferative activities against RT112 bladder cancer cell line and FGFR3 inhibitory activities were tested.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-454**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

New Production of Bioactive Halogenated Polyketides by the Marine-Mudflat-Derived Microorganisms

손병화* 윤금자

부경대학교 화학과

Marine-derived microorganisms continue to attract attention as a rich source of structurally novel bioactive metabolites that are potential lead compounds for the development of new drugs.[1] When the marine-derived microorganisms were cultured under saline condition, they rarely produced interesting biological halogenated metabolites (e.g., salinosporamide A3 of a highly potent inhibitor of the 20S proteasome and its halogenated derivatives).[2] Encouraged by the detection of halogenated marine analogs, we manipulated the fermentation of Marine-mudflat-derived bacteria and fungi by the addition of metal halides in an effort to gain access to a wider cross-section of halogenated secondary metabolites. This presentation describes the production, isolation, and identification of halogenated polyketides, We also show the biological activity of new compounds. 1. Jensen, P. R.; Fenical, W. “Marine microorganisms and drug discovery: current status and future potential”, In “Drugs from the Sea”, (ed Fusetani, N.) pp. 6–29 (Karger, Basel, 2000).2. Lam, K. S.; Tsueng, G.; McArthur, K. A.; Mitchell, S. S.; Potts, B. C. M.; Xu, J. J. Antibiot., 2007, 60, 13–19.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-455**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enzyme responsive sequence modified PAMAM dendrimer for enhanced gene delivery carrier

이슬기 최준식*

충남대학교 생화학과

In the gene delivery system, Poly(amidoamine)(PAMAM) dendrimer has been used as an ideal polymeric carrier. PAMAM dendrimer have branched structure with 64 amine residues and studied for different applications such as drug, imaging agent and gene delivery. In this study, PAMAM Generation 4 - Glycine-Leucine-Phenylalanine-Glycine(GLFG)-Histidine-Arginine was designed for novel gene delivery carrier to enhance transfection efficiency. Oligopeptide GFLG was selectively cleaved by enzyme cathepsin B in the lysosome compartment and His and Arg were modified for proton sponge effect and cell uptake, respectively. PAMAM G4-GLFG-H-R was confirmed to form complex with plasmid DNA at 1:8 (Polymer : pDNA) weight ratio. This polyplexes were measured using dynamic light scattering (DLS). Enzymatic release test shown that complex of G4-GLFG-H-R was collapsed by enzyme Cathepsin B. Luciferase assay has shown remarkably higher transfection efficiency compared with only PAMAM G4 in HeLa cells. This PAMAM G4 based polymeric carrier is emergent nano-carrier and could be useful for biological application and treatment of diseases

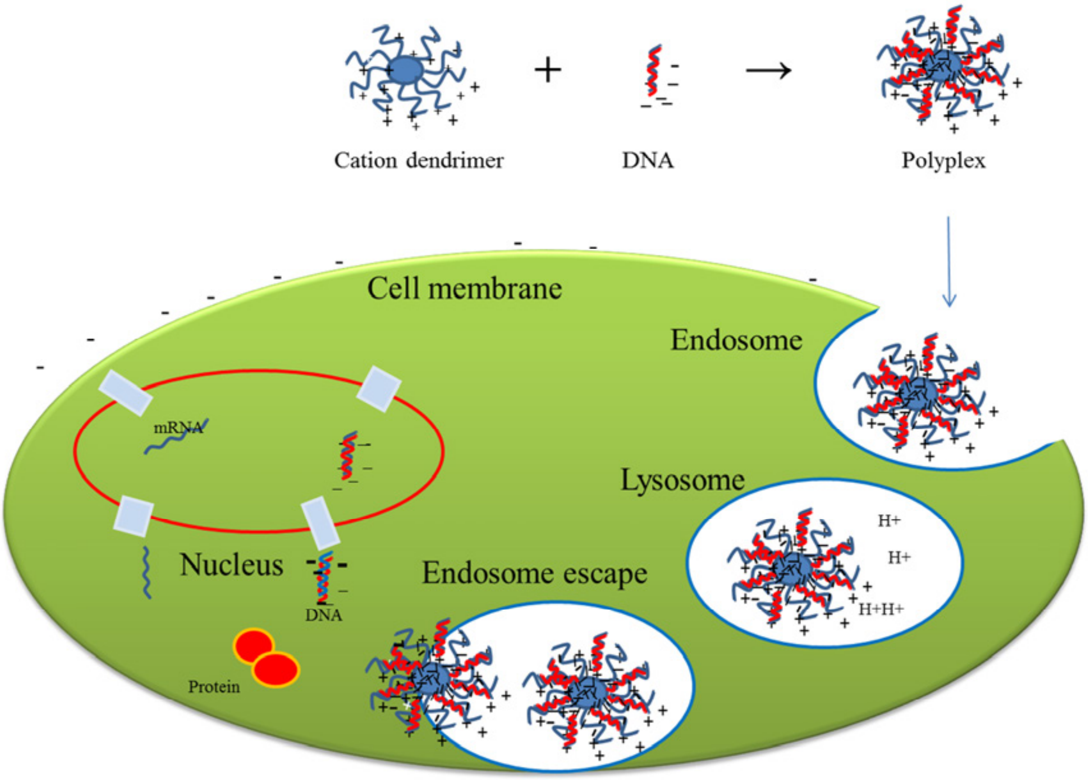
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-456**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced gene delivery effects of PAMAM dendrimer by surface modified with short oligopeptides

LE THI THUY 최준식*

충남대학교 생화학과

Recently, non-viral vectors have become a popular research topic in the field of gene therapy. In this study, we conjugated short oligopeptides to polydoamine-generation 4 (PAMAM G4) to achieve higher transfection efficiency. Previous reports have shown that the PAMAM G4-histidine (H)-arginine (R) dendrimer enhances gene delivery by improving cell penetration and internalization mechanisms. Therefore, we synthesized PAMAM G4-Hphenylalanine (F) R, PAMAM G4-FHR and PAMAM G4-FR derivatives to determine the best gene carrier with the lowest toxicity. In this study,PAMAM G4 derivatives conjugated to H, R, and F were synthesized with a conjugation yield of ≥90%. A complete DNA condensation was achieved, and we obtained nano-sized polyplexes, which were further analyzed in vitro. The suggested acid-base titration profile improved the buffering capacity of the H residue, thereby synergistically inducing early endosomal escape. The higher cellular internalization was confirmed by confocal microscopy and is probably attributable to a greater interaction between the hydrophobic F residue and the cell membrane. Moreover, the PAMAM G4 derivatives exhibited a lower toxicity than that of the PEI 25kD, which makes them safer non-viral gene carriers with a similar level of transfection efficiency. In summary, the PAMAM G4 derivatives are highly promising candidates for gene delivery because of their low toxicity, improved buffering capacity, and higher transfection efficiency.Therefore, our results show that these carriers are promising and may help in achieve higher transfection with negligible cytotoxicity.


Cation dendrimer
+
DNA
→
Polyplex
Cell membrane
Endosome
Lysosome
H+
H+
H+H+
mRNA
Nucleus
DNA
Endosome escape
Protein

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-457**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of UPLC Methods for the Simultaneous Analysis of Anti-diabetic Compounds

윤창용 김남숙 김규연 류금주 이지현 박성관 백선영*

식품의약품안전처 첨단분석팀

According to increasing demand of consumer on well-being, the health functional food market has been growing steadily and globally. In addition, it have been reported that unapproved substances were illegally added in food for enhancing the certain pharmacological efficacy of health functional food without label. Thus, the health of consumers may be able to be exposed at the side effects from those products. Therefore, development of advanced analytical methods is needed to detect unauthorized substances from the tampered food products, rapidly and accurately. The purposes of this study were development and validation of a simutaneous analytical method for detecting anti-diabetic compounds. An ultra performance liquid chromatography (UPLC) was applied for development of the simultaneous analysis for 26 anti-diabetic compounds (Glibenclamide, glipizide, metformin, tolbutamide, etc.). Selectivity, limit of detection (LOD), limit of quantitation (LOQ), linearity and recovery wre carried out for the method validation. All of 26 anti-diabetic compounds were separated with excellent resolution (over 1.5). LODs (spiked in solid sample, 0.10-1.70 μg/mL; spiked in liquid sample, 0.10-1.25 μg/mL) and LOQs (spiked in solid sample, 0.30-5.10 μg/mL; spiked in liquid sample, 0.30-3.75 μg/mL) wre measured, respectively. This method has acceptable recovery values (80.00-110.00%) and linearities ($R^2>0.99$). These results indicated that the proposed method was suitable for application on complex food matrices. Therefore, this study may be helpful to protect the public health as the method to monitor illegal food products.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-458**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of 1H-benzo[d]imidazole-2-thiol Derivatives by using Carbon Disulfide Linker on Solid-Phase

윤효정 공영대*

동국대학교 화학과

Solid-phase Organic Synthesis (SPOS) is routinely used to prepare drug-like, small organic molecules in medicinal chemistry areas. In this experiment, we constructed N-alkyl-1H-benzo[d]imidazole-2-thiol derivatives on solid-phase synthesis. Substituted 1,2-phenylenediamine was used as a starting material and protected with Boc group followed by reaction with carbon disulfide in the presence of triethylamine (TEA) in tetrahydrofuran (THF) to afford 2-mercaptobenzimidazole core skeleton. Next, we loaded 2-mercaptobenzimidazole to the Merrifield resin as a polymer support. With the 2-mercaptobenzimidazole resin in hand, we deprotected Boc group and then introduced various alkyl groups at the Boc deprotected amine position. Finally, our desired product was successively obtained via cleavage reaction with benzyl thiol and potassium tert-butoxide in dimethylformamide (DMF) in high yields and good purities.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-459**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solid-Phase Parallel Synthesis of N-Substituted-2-aminothiazolo[4,5-b]pyrazine Derivatives via Tandem Reaction of Isothiocyanate Terminated Resin with o-Halo-2-Aminopyrazines

ABDILDINOVA AIZHAN 공영대*

동국대학교 화학과

A novel solid-phase synthesis methodology of N-substituted-2-aminothiazolo[4,5-b]pyrazine derivatives was developed. The key step in this synthesis strategy is the tandem reaction of isothiocyanate terminated resin with o-halo-2-aminopyrazine, affording cyclized 2-aminothiazolo[4,5-b]pyrazine resin. To increase the diversity of our library, Suzuki coupling reaction was performed. Further functionalization of 2-aminothiazolo[4,5-b]pyrazine core skeleton with various electrophiles such as alkyl halides, acyl chlorides, and sulfonyl chlorides and cleavage from the resin with TFA in DCM generated N-alkyl-, N-acyl-, and N-sulfonyl-2-aminothiazolo[4,5-b]pyrazine derivatives. The physicochemical properties and the polar surface areas of synthesized compounds were evaluated. This synthetic strategy can efficiently provide a library of small drug-like compounds with potential drug-like properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-460**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of Inventive N-substituted 2-Aminobenzo[d][1,3]thiazine Derivatives on the Solid-Phase Synthesis through BAL-based Resin

전희구 공영대[*] 이은실[1]

동국대학교 화학과 [1]동국대학교 의약화학연구실

A expeditious solid-phase methodology has been developed for the synthesis of N-acyl and N-sulfonyl substituted 2-aminobenzo[d][1,3]-thiazine derivatives. The key step in this methodology is the preparation of backbone amide linker-bonud 2-aminobenzo[d][1,3]-thiazine resin through cyclization reaction of isothiocyanates using the BOMBA resin under microwave irradiation. This core skeleton 2-aminobenzo[d][1,3]-thiazine resin undergoes functionalization reaction with various electrophiles, such as acid halides and sulfonyl halides, to generate N-acyl and N-sulfonyl substituted 2-aminobenzo[d][1,3]thiazine resins, respectively. Finally, N-acyl and N-sulfonyl substituted 2-amino-benzo[d][1,3]thiazine derivatives are generated in good yields and purities by cleavage of the respective resins under trifluoroacetic acid (TFA) in dichloromethane (DCM).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-461**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solid-phase Synthesis of 1,3,4-Oxadiazole Derivatives through Desurfurative Cyclization of Thiosemicarbazide Intermediate Resin

하지은 공영대*

동국대학교 화학과

Heterocyclic compounds have been used as scaffolds on which pharmacophores are arranged to provide potent and selective drugs. This is especially true for five-membered ring heterocyclic compounds, which serve as the core components of many substances that possess a broad range of intriguing biological activities. In this family, 1,3,4-oxadiazoles have been considered as “privileged” scaffolds to produce substances of interest in numerous therapeutic areas, such as anti-inflammatory, anti-microbial, anti-convulsant, anti-cancer, and anti-hypertensive. In this reason, we investigated to establish synthetic methodology for the construction of 1,3,4-oxadiazole analogues. The 1,3,4-oxadiazole core skeleton was successively afforded through desurfurative cyclization of thiosemicarbazide derived from a reaction between isothiocyanate and hydrazide. Finally, the resulting 1,3,4-oxadiazole was easily diversified by substitution, and Suzuki-coupling reaction in good yields and high purities.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-462**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solid-phase Synthesis of 1,3,4-Thiadiazole Analogues Through Desulfurative Cyclization of Thiosemicarbazide Intermediate Resin

양승주 김강태 공영대*

동국대학교 화학과

In this experiment, we developed a solid-phase synthetic method to construct a 1,3,4-thiadiazole library. This method involves the preparation of polymer-bound 2-amido-5-amino-1,3,4-thiadiazole resin through cyclization of thiosemicarbazide resin by using the p-TsCl as a desulfurative agent and then the resin was functionalized by alkylation, acylation, alkylation/acylation, and Suzuki coupling reaction. The alkylation reaction and acylation reaction chemo-selectively occurred at 2-amide position of 2-amido-5-amino-1,3,4-thiadiazole resin and 5-amine position of 2-amido-5-amino-1,3,4-thiadiazole resin, respectively. Furthermore, we calculated physicochemical and biological properties of 1,3,4-thiadiazole derivatives. As a result, 1,3,4-thiadiazole derivatives showed good physicochemical and biological properties in a range of bioavailable drug property by Lipinski's Rule and parameters.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-463**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of 1-Alkyl/Acyl/Sulfonyl-2-aminobenzo[d]imidazole Derivatives via Desulfurative Cyclization on Solid-phase Organic Synthesis

유현정 공영대*

동국대학교 화학과

In this study, we synthesized 1-alkyl/acyl/sulfonyl-2-aminobenzo[d]imidazole derivatives. 2-Fluoronitrobezene was used as a starting material and reacted with various amines followed by reduction reaction of nitro group to afford alkyl substituted 1,2-phenylene diamines. The alkyl substituted 1,2-phenylene diamine reacted with polymer supported isothiocyanate derived from 4-benzyloxy-2-methoxybenzylamine (BOMBA) resin through a reaction with carbondisulfide, trimethylamine and p-TsCl in tetrahydrofuran (THF) to generate thiourea intermediate resin. The cyclization of thiourea intermediate resin was successfully conducted through desulfurative cyclization with 2-chloro-1,3-dimethyimidazolinium chloride (DMC) and N,N-diisopropylethylamine in dichloromethane (DCM). Next, various electrophiles such as alkyl halides, acid chlorides and sulfonyl chlorides were used to functionalize 2-amine position. Finally, we obtained various 1-alkyl/acyl/sulfonyl-2-aminobenzo[d]imidazoles by cleavage of the corresponding resin under trifluoroacetic acid (TFA) in dichloromethane (DCM).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-464**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation and characterization of glycol chitosan-graft-polyethylenimine/pDNA complexes

이영화 최준식*

충남대학교 생화학과

A glycol chitosan-based polymer that spontaneously assembles with plasmid DNA into nanorods was evaluated as a non-viral vector for gene delivery. Glycol chitosan–methyl acrylate-polyethylenimine(GMP) was synthesized by grafting polyethylenimine onto glycol chitosan via amidation after Michael addition using methyl acrylate. Gel retardation and PicoGreen assay experiments showed complete complex formation with plasmid DNA. GMP/pDNA complexes were characterized using biophysical tech-niques and were found to be positively charged rod-shape structures with widths in the nanometer scale and lengths in the micrometer scale. Transfection efficiency and cytotoxicity of GMP polymer was evaluated in human epithelial ovary carcinoma (HeLa) cells, human embryonic kidney 293 (HEK293)cells, and human hepatocellular liver carcinoma (HepG2) cells, in comparison to high molecular weight polyethylenimine, a commonly used transfection reagent. Intracellular polymer uptake was compared and confirmed by confocal microscopy. The results demonstrate that GMP, a hybrid polymer of glycol chitosan grafted with branched polyethylenimine, may serve as a promising vehicle for efficient gene delivery.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-465**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Automated radiosynthesis of ^{18}F-radioligand for brain PET imaging of glutamatergic system

전중현* **박준영[1]** **손정민[1]** **윤미진** **CHOARTHUREUNGHYUCK**

연세대학교 의과대학 핵의학교실 [1]연세대학교 의과대학 핵의학과

The impact of mental disorders such as depression and other neurodegenerative diseases on the mortality of patients implies an unmet need for action in neuroscience. The glutamatergic system consisted of ionotropic ligand-gated cationic channels and metabotropic glutamate receptors have shown many implications in mental disorders. Among those, the metabotropic glutamate receptor subtype 5 (mGlu5) has emerged as attractive therapeutic target due to its implication in pathophysiology of psychiatric and neurological disorders such as depression, addiction, Parkinson`s disease, Fragile X syndrome and inflammatory pain. Herein, we wish to report the automated radiosynthesis of ^{18}F-PSS232 radiotracer for brain PET imaging for mGlu5. ^{18}F-PSS232 was prepared on the GE TracerLab Fxn module with computer-programmed sequences. Nucleophilic fluorination of mesylate (-OMs) group on the (*E*)-PSS232-OMs with cyclotron-produced fluoride ion at 100 ^{o}C in DMF, followed by HPLC purification and formulation gave ^{18}F-(*E*)-PSS232 in 15-21 % radiochemical yield (decay-corrected, n=5) at the end of synthesis (EOS) with radiochemical purity (RCP) above 95 % for ^{18}F-(*E*)-conformer. Specific activity was determined to be in the range between 37–54 GBq/μmol. Further development of these procedures includes the establishment of a robust and reliable radiosynthesis to meet the GMP regulation is in progress. The potential radiotracer, ^{18}F-PSS232, for the human glutamatergic system predominantly using PET studies would help to understand the neurochemical defects within the brain using newly-developed mGlu5 PET ligand. This work was supported by NRF, funded by the Ministry of Science of Korea (2015K1A3A1A14021182).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-466**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design and Synthesis of new substituted pyrimidines as potential anticancer agents

백소라 노은주[1,*]

경희대학교 기초약학과 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

In this work, we report design and synthesis of fifteen derivatives of pyrimidine scaffold as potential anticancer agents. The detailed synthetic scheme is reported as well as the rational design of the new series. Biological evaluation of our compounds has been performed in Reaction Biology co. Four compounds have demonstrated good inhibitory activity against EGFR and/or HER2 receptors. From our results, we report compound KKRE9408 as the most promising EGFR/HER2 inhibitor anticancer potential candidate.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-467**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design of the Well-Defined Antibody-Drug Conjugates (ADCs) :Preclinical Development of an anti-HER2 ADC, LCB14-0110

김형래

(주)레고켐 바이오사이언스 chemistry

LegoChem Biosciences has developed a novel, next-generation site-specific antibody-drug conjugates (ADCs) platform technology called ConjuallTM which enables the generation of homogenous ADCs with specifically defined number of payload only at the intended sites on the antibody employed. This presentation will also illustrate a novel linker chemistry that showes superb plasma stability. With the result, we have developed preclinical candidate, LCB14-0110 which is highly efficacious, site-specific, and plasma-stable anti-HER2 ADC.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-468**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design and Synthesis of novel pyrazolo[3,4-*d*]pyrimidin-1-yl piperidine derivatives as Bruton's tyrosine kinase inhibitors

박혜빈 황종연[1,*] 윤창수[1,*] 김필호[1,*] 정희정[1,*] 류도현 조성윤[2]

성균관대학교 화학과 [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 난치성질환치료제 연구센터

Bruton's tyrosine kinase (BTK), a non-receptor tyrosine kinase, plays an important role in the B cell receptor signal transduction pathways regulating activation, survival, proliferation, and differentiation of B-lineage lymphoid cells. Mutations in gene encoding human BTK lead to X-linked agammaglobulinemia (XLA) in humans and X-linked immunodeficiency (Xid) in mice. Aberrant activation of BTK is implicated with the pathogenesis of B cell lymphoma because B cells play a central role in the pathogenesis of several autoimmune diseases and B cell malignancies. Indeed, inhibition of BTK has been considered as an effective and attractive therapeutic target for B cell related malignancies. In this report, we synthesized a series of pyrazolo[3,4-*d*] pyrimidine derivatives that were substituted with diphenyl moieties and evaluated BTK kinase inhibitory activity and cell based proliferation assay. Some of the compounds displayed excellent activity in vitro enzymatic and cell-based assay.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-469**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enzyme-responsive destabilization of stabilized plasmid-lipid nanoparticles as an efficient gene delivery

송수정 이슬기 최준식*

충남대학교 생화학과

Stabilized plasmid lipid nanoparticles (SPLPs) have been developed to overcome the low stability issue of cationic liposomes, however, SPLPs that are too stable result in unsatisfactory transfection efficiency. In this article, we prepared enzyme-responsive SPLPs (eSPLPs) composed of 1,2-dioleoyl-3-trimethylammonium-propane (DOTAP), 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE), and mPEG-GLFG-K-(C16)2, a PEG lipid with an enzymatically-cleavable linker (glycine-phenylalanine-leucine-glycine, GFLG). eSPLPs were successfully prepared with a pDNA encapsulation efficiency of over 80%, using the detergent dialysis method. The PEG shell stabilized the eSPLPs and maintained a hydrodynamic diameter of 200 nm, however, in endosomal conditions, cathepsin B degraded the GFLG linker, decoating the PEG shell from the eSPLPs. Decoated eSPLPs were rapidly destabilized, and induced endosomal disruption in order to the encapsulated pDNA to escape into the cytosol. Owing to the cathepsin B-responsive destabilization, the eSPLPs showed a 10 to 100-fold higher transfection efficiency than normal SPLPs, which was confirmed using luciferase assay. These results suggest that eSPLPs are a promising candidate for use as a practical gene delivery carrier, with both stability and high transfection efficiency for future in vivo applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-470**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Chemiverse BOILED-Egg: The QSAR Models to Predict HIA and BBB permeability

서용일* 남기엽 서영주 강경태 김민경 윤정혁[1]

(주)파로스아이비티 바이오인공지능연구소 [1](주)파로스아이비티 -

In previous study, Gastrointestinal absorption and brain access are two pharmacokinetic behaviors crucial to estimate at various stages of the drug discovery processes. The reason why many drug development failures are imputable to poor pharmacokinetics and bioavailability except of efficacy and toxicity. The many models proposed to human intestinal absorption (HIA) and blood–brain barrier (BBB) permeability correlated with the n-octanol/water partition coefficient (log P) and the polar surface area (PSA). Recently, a new model suggested to predict HIA and BBB developed by A. Daina et al. called the Brain Or IntestinaL EstimateD permeation method (BOILED-Egg). The BOILED-Egg model was described by the lipophilicity and polarity, too: The log P method developed by Wildman and Crippen (WlogP) was chsosen and the topological polar surface area (tPSA). In this study, we compare the predicatability of BOILED-Egg model based on different logP methods, e.g., AlogP98, SlogP, and SKlogP. In addition, we reproduced BOILED-Egg model to predict the HIA and BBB with various logP models. If you want to predict HIA or BBB with your compounds, you can freely evaluate in our drug discovery platform (http://www.chemiverse.co.kr).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-471**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design, synthesis, molecular modeling and biological evaluation of novel CSF1R inhibitors based on pyrimidine scaffold

Ahmed Karam Mohamed 노은주[1,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

CSF1R (namely; FMS) is a protein tyrosine kinase that is exclusively expressed in monocyte-macrophages and belongs to the PDGFR family of type III receptor tyrosine kinases and was first discovered as the oncogene responsible for Feline McDonough Sarcoma. A small molecule FMS inhibitor was found to slows the progression of amyotrophic lateral sclerosis, prevent erosions, reduce symptoms of RA and bone osteolysis. In this study we report the design of novel 2,5-diaminopyrimidine derivatives to selectively inhibit FMS. 5 compounds were designed, synthesized and assayed over FMS kinase. Compound 1 showed sub-nanomolar IC50 against FMS. Kinase panel was made to confirm the selectivity of compound 1. Molecular docking study was carried out to predict the possible binding mode of the new compounds with the FMS kinase. The molecular docking study demonstrated the favorable binding modes of the novel compounds in the ATP-binding pocket of FMS.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-472**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of pyrazolo[3,4-d]pyrimidine derivatives for polo-like kinase 2 inhibitor evolution

함미숙 정규성 정찬성[1,*]

연세대학교 화학과 [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

Among several families of protein kinases which have shown a critical role in the regulation of cell cycle progression, the Polo-like kinases have been widely studied as a cell cycle regulator including entry into mitosis and cytokinesis, also are key players in DNA replication and DNA damage response. Owing to their essential involvement in cell cycle regulation, the Polo-like kinase family has emerged as an attractive therapeutic target in oncology. In this poster, we discuss the progress in the development of small-molecule inhibitor for Plk2 which is subunit of Plk family. In our early screening process, some compounds of pyrazolo[3,4-d]pyrimidine scaffold exhibited high selective activity for Plk2 and were required to tune finely. To do this goal, their derivatives were synthesized by alkylation and cyclization through modifying C3, C6 site of pyrazolo[3,4-d]pyrimidine. Especially, the sulfone group substitution with nitrile ion in the pyrimidine ring will open the door for the diversification of these compounds to get the improved biological activity. During these investigations, we will discuss the synthetic and analytical methods of pyrazolopyrimidne analogues and biological results as well.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-473**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

유방암 진단용 I-124 표지 유/무기 하이브리드 나노구조체의 합성 및 생물학적 평가

이준영 박정훈 허민구 양승대*

한국원자력연구원 방사선기기연구부

안쓰라퀴논 유도체인 Rhein 은 에스트로겐 수용체를 타겟팅 할 수 있는 유기화합물로서 각종 암의 진단 및 치료제로 이용되고 있는 금 나노입자와 간단한 과정으로 합성이 가능하다. 유방암에 과발현 되어있는 에스트로겐 수용체와 Rhein 의 친화도를 통해 PET 용 이미징 시약으로서 사용 가능 할 것이다. 본 연구에서는 나노 캐리어와 치료용으로서 금 나노입자를 도입하였으며, 타겟 물질로 I-124 가 표지 된 Rhein 을 사용하여 유/무기 하이브리드 나노구조체를 합성하였다. 암세포의 식세포 작용에 용이한 사이즈인 30 nm 의 금 나노입자는 citrate 환원제를 사용하여 합성하였으며, linker 로서 carbodiimide coupling 방법으로 L-cysteine 을 도입하였다. 금 나노입자와 Rhein-cystein 은 2 분간 초음파 처리하여 합성 하였으며, Chloramine T 를 산화제로 사용하여 I-124 을 표지 하였다. 유/무기 나노구조체의 분리 및 정제는 원심분리를 통해서 진행하였다. [^{124}I]Rhein-Cys-Au 의 방사화학적 수율은 65% ± 8.2%이며, >98%의 방사화학적 순도로 합성 되었다. [^{124}I]Rhein-Cys-Au 나노구조체의 세포섭취도 평가는 에스트로겐 수용체가 과발현 되어있는 유방암 세포주인 MCF-7 을 대상으로 진행 하였으며, 그 결과로는 호르몬에 의존해서 시간에 따라 증가하는 경향을 보였다 (15 min: 25.4 ± 1.59%, 30 min: 27.1 ± 1.27%, 60 min 28.6 ± 0.38%, 120 min: 15.97 ± 0.66%). 또한, MCF-7 이 이식된 마우스의 PET 측정을 통해서 유방암에 대한 상당한 친화도를 확인하였다. 이를 토대로 유방암에 대한 진단용 PET 이미징 시약으로서 사용 가능할 것으로 보여지며, 차후 금 나노입자의 방사화를 통해 유방암의 진단 및 치료를 동시에 할 수 있을 것으로 기대 된다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-474**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design and synthesis of chalcone-templated Heat shock protein 90 inhibitor and their effects on gefitinib resistance in non-small cell lung cancer (NSCLC)

최명아 서영호[1,*]

계명대학교 약학과 [1]계명대학교 약학대학

Non-small cell lung cancer (NSCLC) is the most common type of lung cancer and that is responsible for 85% of lung cancer patients. Despite several EGER inhibitors have been developed in the treatment of NSCLC, the clinical efficacy of EGFR inhibitors in NSCLC is limited by the development of drug-resistance through the mutation of EGFR and the overexpression of Met. Considering both EGFR and Met are client proteins of Hsp90, blocking Hsp90 folding machinery may be best suited to overcome the resistance form EGFR mutation and Met amplification. Heat shock protein (Hsp90) is an ubiquitous molecular chaperone protein, which accounts for 1-2% of the cytosolic protein under non-stressed conditions. Hsp90 plays an important role in regulating maturation and stabilization of many oncogenic proteins in ten essential hallmarks of cancer. Its client proteins include EGFR, Her2, Met, Akt, Raf, HIF-1, and MMP2. Hsp90 is overexpressed in tumor cell more than normal cell. Hsp90 inhibitor can lead to the degradation of a large collection of oncogenic proteins. In this regard, Hsp90 represents great promise as a therapeutic target of cancer due to its potential to simultaneously disable multiple signaling pathways. In this study, we designed and synthesized a number of inhibitors and they disrupted Hsp90 chaperoning function and impaired the growth of gefitinib-resistant non-small cell lung cancer (NSCLC). The result suggested that these compounds could serve as a potential lead compound to overcome the drug resistance in cancer chemotherapy.

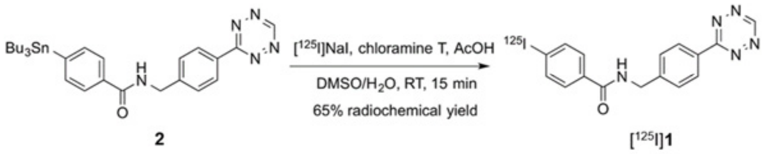
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-475**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

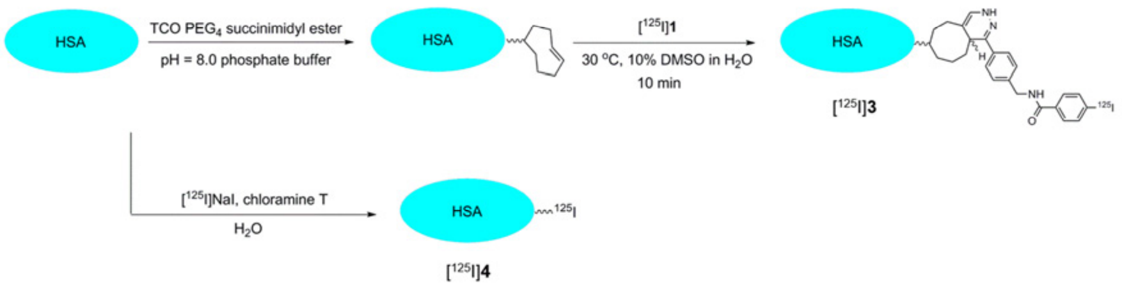
Radiosynthesis of ^{125}I-labeled tetrazine for rapid and efficient radiolabeling of biomolecules using inverse-electron-demand Diels-Alder reaction

심하은 최미희 윤성재 이창헌[1] 장범수 이효선[2] 전종호[3,*]

한국원자력연구원 생명공학연구부 [1]한국원자력연구소 생명공학연구부 [2]경북대학교 자연과학대학 화학과 [3]한국원자력연구원 첨단방사선연구소

In this study, we present a rapid and efficient radiolabeling method of trans-cyclooctene (TCO) group containing molecules using ^{125}I-labeled tetrazine prosthetic group. For this study, radioiodination of the stannylated precursor 2 was carried out using [^{125}I]NaI to give ^{125}I-labeled tetrazine ([^{125}I]1) with high radiochemical yield (65±8%) and radiochemical purity (>99%). TCO group conjugated human serum albumin (HSA) was reacted with [^{125}I]1 under mild condition to give the radiolabeled products [^{125}I]3 with an excellent radiochemical yield (>99%). We next carried out the tissue biodistribution study of [^{125}I]3 in normal ICR mice to investigate the level of organ accumulation profile. The biodistribution study of [^{125}I]3 showed significantly lower thyroid uptake values compared with ^{125}I-labeled HSA ([^{125}I]4) prepared by a traditional iodine labeling protocol using chloramine T method. Therefore [^{125}I]3 will be used as a quite useful radiotracer for the various biomedical and imaging study. These results clearly indicated that the present radiolabeling method using inverse-electron-demand Diels-Alder reaction would be useful for radioactive iodine labeling of TCO group conjugated biomolecules.


Bu3Sn
H
N
O
N
N
N
N
2
[125I]NaI, chloramine T, AcOH
DMSO/H2O, RT, 15 min
65% radiochemical yield
125I
H
N
O
N
N
N
N
[125I]1


HSA
TCO PEG4 succinimidyl ester
pH = 8.0 phosphate buffer
HSA
[125I]1
30 °C, 10% DMSO in H2O
10 min
HSA
NH
N
H
NH
O
125I
[125I]3
[125I]NaI, chloramine T
H2O
HSA
125I
[125I]4

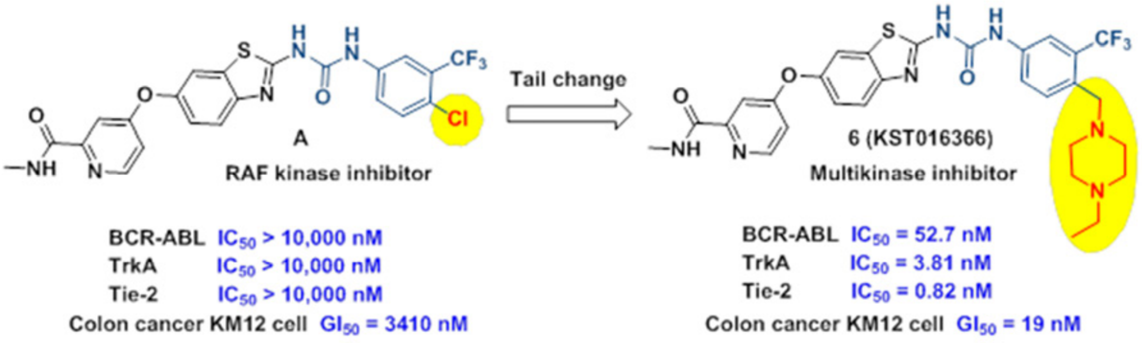
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-476**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

KST016366: An orally active antiproliferative agent with multiple kinase inhibitory activity including the angiogenic VEGFR /Tie2 and oncogenic TrK kinases

<u>ELDAMASY ASHRAF KAREEM AWAD MOHAMMED</u> 금교창[1,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) 케모인포메틱스연구센터

Herein, we report the discovery of compound KST016366 as a new potent multikinase inhibitor through minor structural modification of our previously reported RAF kinase inhibitor A. In vitro anticancer evaluation of 6 showed a substantial broad spectrum of antiproliferative activity against 60 human cancer cell lines. In particular, it showed GI50 values of 51.4 nM and 19 nM against leukemia K-562 and colon carcinoma KM12 cell lines, respectively. Kinase screening of KST016366 displayed its multiple kinase inhibitory activity in nanomolar scale over certain oncogenic kinases implicated in cancer tumorigenesis as well as angiogenesis. Interestingly, it displayed IC50 values of 0.82 nM, 3.81 nM and 53 nM over Tie2, TrkA and ABL-1 (wild and T315I mutant) kinases, respectively. Moreover, KST016366 is orally bioavailable with a favorable in vivo PK profile. Compound KST016366 may serve as a promising candidate for further development of potent anticancer chemotherapeutics.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-477**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Quinolone and Coumarin derivatives as inhibitors of TTR amyloidogenesis and fluorescent sensors

이슬기 최성욱[1,*]

충남대학교 신약개발학과 [1]충남대학교 신약개발학과

Amyloid fibril formation has been associated with a wide range of diseases, such as Alzheimer's disease. Transthyretin (TTR) is one of the proteins generating amyloid fibrils. TTR is a homotetrameric protein composed of 127-amino-acid, β-sheet-rich subunits. The established physiological functions of TTR are to bind to and transport the thyroid hormone thyroxine (T4) and holo-retinol binding protein in the blood and cerebrospinal fluid (CSF).Tetrameric TTR may dissociate to a non-native monomer that cause or suppress misfolding and/or misassembly. These results lead to amyloidoses due to proteotoxicity and cell degeneration.Dissociation of the tetramer is thought to be a prerequisite for amyloid formation in vitro and involvement of monomers and/or dimers in fibril formation has been suggested. Small molecules that bind to T4 binding site stabilize the ground state of tetrameric TTR and raise the kinetic barrier for dissociation, imposing kinetic stabilization on TTR and preventing aggregation.Herein we synthesized and evaluated the possibility of compounds as potent inhibitors of TTR amyldoidogenesis and as fluorescent sensors for tetrameric TTR to measure a concentration of TTR in human plasma.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-478**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Treatment of Sepsis Pathogenesis with High Mobility Group Box Protein 1-regulating Anti-Inflammatory Agents

조완상 박승범*

서울대학교 화학부

Sepsis is a high risk symptom often associated with multiple organ failure, of which a mortality rate of almost 20%. However, due to the diverse patterns of sepsis pathogenesis, there are a huge lack of proper therapy for sepsis. The pro-inflammatory cytokine cascade is on the underlying basis of sepsis progression. As a late stage pro-inflammatory cytokine, the role of high mobility group box protein 1 members (HMGBs) in regulating cytokine cascade has emerged. We previously reported on the novel small-molecule modulator, inflachromene (ICM), which inhibits the release of HMGBs. ICM successfully reduces the production of pro-inflammatory cytokines in BV-2 microglia. In this context, we administered ICM by i.p. injection to a cecal ligation and puncture (CLP)-induced mouse model of sepsis. We could observe that ICM successfully ameliorated sepsis. Based on the structure-activity relationship study, we discovered new candidate compounds, 2j and 2l, and they showed improved therapeutic efficacy in an in vivo mouse model of sepsis. From these observations, this study clearly demonstrates that the regulation of HMGB1 release with the small molecule is a promising therapeutic strategy for sepsis.

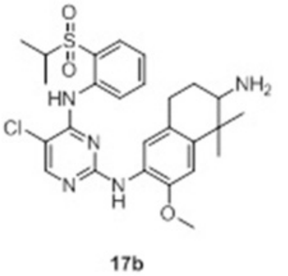
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-479**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of novel 2,4-diaminopyrimidines bearing tetrahydronaphthalenyl moiety as ALK inhibitor

이동호 김필호[1] 김형래[2] 윤창수[1] 정희정[1] 조성윤[2] 하재두[2] 이덕형 황종연[1,*]

서강대학교 화학과 [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 난치성질환치료제연구센터

Abstract A series of novel 2,4-diaminopyrimidines bearing tetrahydronaphthalenyl moiety were synthesized and evaluated for their anti-anaplastic lymphoma kinase (ALK) activities using enzymatic and cell-based assays. Amongst the compounds synthesized, compound 17b showed promising pharmacological results in in vitro, ex vivo, and pharmacokinetic studies. An in vivo efficacy study with compound 17b demonstrated highly potent inhibitory activity in H3122 tumor xenograft model mice. A series of kinase assays showed that compound 17b inhibited various kinases including FAK, ACK1, FGFR, RSK1, IGF-1R, among others, thus demonstrating its potential for synergistic anti-tumor activity and development as a multi-targeted non-small cell lung cancer (NSCLC) therapy.



17b

ALK wt	IC_{50} = 0.7 nM
L1196M	IC_{50} = 1.5 nM
H3122	CC_{50} = 16 nM
Ba/F3 L1196M	CC_{50} = 62 nM

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-480**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Xanthotoxol Derivatives for Cholinesterase Inhibitors

전철민[*] 박경찬[1] 신수정[2] 이하늘 박정호[3,*]

한밭대학교 화학생명공학과 [1]한밭대학교 생명공학과 [2]한밭대학교 응용화학과 [3]한밭대학교 응용화학생명공학부

Cholinesterase (ChE) inhibitors and N-Methyl-D-aspartate (NMDA) receptor antagonist such as tacrine, donepezil, rivastigmine, and galantamine are clinically approved to treat Alzheimer's disease (AD) patients, but new therapeutic compounds are still needed to be developed. Since inhibition of cholinesterase (ChE) is still considered to be one of the most effective targets to treat Alzheimer's disease (AD) patients, we have tried to synthesize many new classes of ChE inhibitors. In an effort of identifying new type of cholinergic drug, the xanthotoxol derivatives were synthesized and their anticholinesterase effect were evaluated. Xanthotoxol is one of the major active component in *Cnidium monnieri*. It have a furanocoumarin moiety and possess a neuroprotective effects. It was synthesized by the demethylation reaction of xanthotoxin treated with BBr3. The best inhibitor among the triazole-containing xanthotoxol derivatives synthesized from the Click reaction is 5-(1,2-dithiolan-3-yl)-N-(2-(2-(4-(((7-oxo-7,8-dihydronaphtho[2,3-b]furan-9-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)ethoxy)ethyl)-pentanamide (IC_{50} = 6.86 ± 0.33 μM for BuChE). The IC_{50} value of 9-(benzyloxy)-7H-furo[3,2-g]chromen-7-one, which coupled with xanthotoxol and benzyl bromide, is 1.89±1.28 μM for BuChE. It is more effective butyrylcholinesterase inhibitor compared to galantamine (IC_{50}=9.49±2.5 μM).

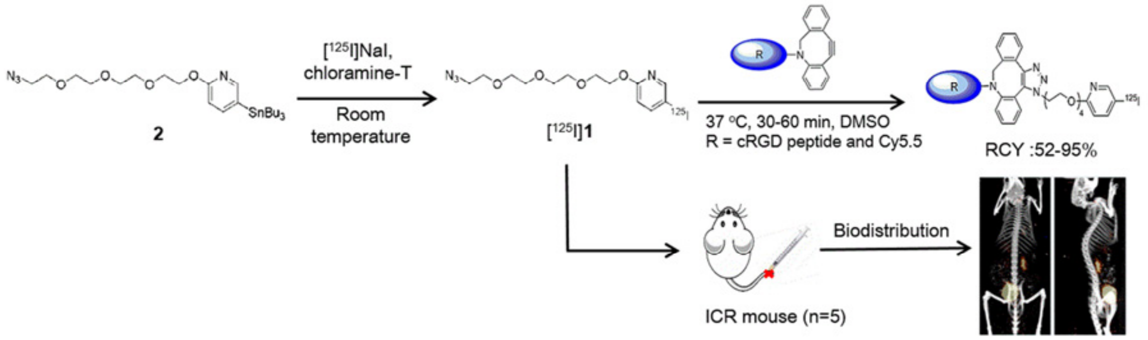
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-481**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Radiosynthesis and *in vivo* evaluation of ^{125}I-labeled azide prosthetic group for efficient radiolabeling of dibenzocyclooctyne conjugated molecules using copper-free click reaction

최미희 심하은 장범수 전종호[1,*]

한국원자력연구원 생명공학연구부 [1]한국원자력연구원 첨단방사선연구소

Copper-free click reaction has been widely used for the bioorthogonal labeling of a variety of biomolecules, cells, and living subjects. Because of the excellent specificity and rapid reaction rate, copper-free click reaction has also been applied to the radiolabeling of biomolecules. Herein, we present an efficient and site-specific radioactive iodine labeling method using copper-free click reaction. For this study, ^{125}I-labeled azide ([^{125}I]1) was synthesized by using a stannylated precursor (2) and [^{125}I]NaI. Observed radiochemical yield and radiochemical purity of the purified product ([^{125}I]1) were 75% and >99% respectively. To evaluate *in vitro* radiolabeling efficiency of [^{125}I]1, dibenzocyclooctyne (DBCO) group conjugated substrates (cRGD peptide and Cy5.5) were prepared. The radiolabeling reactions of these DBCO substrates were performed at 37^{o}C for 30-60 min to give the desired products with modest to good radiochemical yields (52-95%). We next carried out the organ biodistribution study and SPECT imaging of [^{125}I]1 using normal ICR mice for *in vivo* pre-targeted imaging study. As a result, large amount of ^{125}I-labeled azide tracer initially distributed in the liver and kidney and underwent rapid renal clearance. Additionally, [^{125}I]1 was found to be quite stable (>90%) in a mouse serum for 72 h. These results clearly indicated that [^{125}I]1 will be a useful radiotracer for both *in vitro* and *in vivo* radioactive iodine labeling of DBCO group containing molecules.


N_3
2
$SnBu_3$
[^{125}I]NaI,
chloramine-T
Room
temperature
[^{125}I]1
^{125}I
R
37 °C, 30-60 min, DMSO
R = cRGD peptide and Cy5.5
RCY :52-95%
ICR mouse (n=5)
Biodistribution

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-482**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anti-cholinesterase compounds from Mucunae Caulis

이유나[*] 정규선[1] 권희수 이봉호[2,*] 최병욱[*]

한밭대학교 화학생명공학과 [1]한밭대학교 생명공학과 [2]한밭대학교 응용화학생명공학부

In our continuing search for anti-oxidative and anti-cholinesterase compounds from oriental medicinal plant, Mucunae Caulis was examined and here we report the progress on the purification and structural determination of anti-cholinesterase compounds. From the 100% methanol extract of M. Caulis (500g), solvent partition fractions were prepared by using n-hexane(14-MCH), chloroform(14-MCC), butanol(14-MCB), water(14-MCW). Among them 14-MCB showed strong anti-oxidative and BuChE* inhibitory activities. The 14-MCB of M. Caulis showed 94.3% DPPH radical scavenging activity and 70.8% BuChE inhibitory activity at 0.1mg/mL. Using ODS open column chromatography the 14-MCB fraction was separated into 5 fractions(14-MCB-1~5), and each fraction showed anti-oxidative activity as 83.1, 84.7, 81.0, 77.3, 77.4% at 0.1mg/mL, respectively. The 14-MCB-2 fraction was further fractionated into 6 fraction(14-MCB-2-1 ~ 14-MCB-2-6) using ODS column chromatographic method. It was subsequently purified as 14-MCB-2-5-5-3 (3.43mg) and the structure was analylzed by the NMR and MS experiments. Structure determination of 14-MCB-2-5-5-3 and its biological activities will be presented.*BuChE : butyrylcholinesterase

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-483**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anti-cholinesterase compounds from *Grateloupia elliptica*

이유나[*] 최예진 최병욱[*] 이봉호[1,*]

한밭대학교 화학생명공학과 [1]한밭대학교 응용화학생명공학부

In our continuing search for antioxidative and anti-cholinesterase compounds from marine alga, *Grateloupia elliptica* was examined and here we report the progress on the purification and structural determination of anti-cholinesterase compounds. From the 100% ethanol extract of *G. elliptica* (4kg), solvent partition fractions were prepared by using ethanol(NPK003A), butanol(NPK003B) and water(NPK003C). Initial extracts are exhibited low bioactivity. Using various chromatographic methods and by the bioassay-guided fractionation, the NPK003A fraction was separated into seven fractions(NPK003A01 ~ NPK003A07), and each fraction showed BuChE* inhibitory activity as 38.2, 31.5, 49.1, 40.6, 33.1, 23.4, 39.8% at 0.1mg/mL, The NPK003A03 fraction was further fractionated into 5 fractions(NPK003A03a ~ NPK003A03e) using preparative MPLC. NPK003A03a and NPK003A03b showed a significant AChE** inhibitory effect. The NPK003A03b was further purified to give 4 fraction(NPK003A03bF1 ~ NPK003A03bF4) using preparative HPLC. NPK003A03bF2 has shown a high BuChE inhibitory activity and a significant AChE inhibitory activity. Therefore, NPK003A03bF2 may be considered as a target for the next phase with a pure crystal structure. In addition, the most potent activity is NPK003A03bF4 so far, the chemical structure of this is under progress.* BuChE : Butyrylcholinesterase, ** AChE : Acetylcholinesterase

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-484**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of Heat Shock Protein 90 Inhibitors

박선유 서영호[1,*]

계명대학교 약학과 [1]계명대학교 약학대학

Over the past two decades, several targeted drugs have been discovered to eradicate cancers in specific ways and reduce the harmful nonspecific side effects. This “one disease-one target approach” has been prevalent paradigm in pharmaceutical industry and brought about several targeted drugs such as Gleevec (Novartis), Iressa (AstraZeneca) and Herceptin (Genentech). Despite their superiority in their therapeutic efficacy and selectivity, recent evidence has shown that most single-target drugs encounter the emergence of drug resistance in long-term use. In this regard, Heat shock protein 90 (Hsp90) has emerged as an attractive therapeutic target in cancer research. Hsp90 is a molecular chaperone, which plays an important role in cancer cell survival and proliferation by regulating maturation and stabilization of numerous client protein. Most of Hsp90 clients are oncoproteins, including EGFR, Her2, Met, Cdk4, Akt and HIF-1α. Accordingly, the inhibition of Hsp90 function promotes ubiquitin-dependent proteasomal degradation of its client proteins, which can eventually overcome the drug resistance and lead to cell death. In this study, systematic analysis of multiple X-ray cocrystal structures enabled us to design and optimize a novel class of Hsp90 inhibitor. The overall synthetic schemes developed in this study allowde us to easily prepare the intermediates and diverse analogues. In addition, its practical synthetic route makes it readily amenable to large scale synthesis. Compound 19 demonstrated an exceptionally potent binding affinity to the N-terminus of Hsp90• • in •a FP assay. Docking simulation demonstrated that compound 19 tightly occupied ATP-binding pocket in the N-terminus of Hsp90• ; supporting strong binding affinity of compound 19 to Hsp90• •observed in a FP assay. The strong enzyme affinity of compound 19 agreeably translated into good cellular activity, in that compound 19 inhibited the proliferation of H1975 non-small cell lung cancer and Skbr3 breast cancer cell lines. Here, we report our effort to develop therapeutic agents against Hsp90 in cancer.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-485**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structural Design and Biological Evaluation of Pyridone-Based Histone Deacetylase Inhibitors for Recovery of Activation and Stability of RUNX3

국윤정 한균희[1,*]

연세대학교 융합오믹스 의생명과학과 [1]연세대학교 생명공학과

Histone deacetylases (HDACs) have been great research targets for cancer treatment since their aberrant expression due to abnormal epigenetic change was known to play a significant role in tumor onset and progression. Recently, HDAC inhibitors are reported to stabilize a tumor suppressor called runt-related transcription factor 3 (RUNX3) and recover its anticancer activity that is commonly found repressed in various tumor cells. In the previous study, we introduced a new approach to cancer treatment using HDAC inhibitors that restores RUNX3 activity and also presented a series of novel compounds to recover RUNX3 activity.In this study, we reported a new series of HDAC inhibitors by introducing an alkenyl linker between the core and the cap group to improve biological activity and metabolic stability. Through structure-activity relationship (SAR) study, we found that the introduction of an alkenyl group enhanced rigidity of the compound structure, thus facilitating a better fit to the HDAC active site, and increased metabolic stability. We conducted in vitro biological assay to select compounds with high level of activity and metabolic stability. Then, we analyzed in vivo anti-cancer effect of the selected compounds in a xenograft regression model using gastric cancer cell lines. Compound 7k showed the highest inhibition level of tumor growth as a result, so it was selected for further pharmacokinetic evaluation. Showing a high oral bioavailability, compound 7k showed a prospect of being a candidate for anticancer chemotherapeutic agent with high efficacy and metabolic stability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-486**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery and optimization for IRAK4 inhibitor based on the water network analysis

이명휘 OHYOONSUK 조영식[1] 강남숙[*]

충남대학교 신약전문대학원 [1]계명대학교 약학대학

Protein kinase is related to inflammatory disease, cancer, and so on. Because of the well defined structural characteristics of the binding domain. most of kinases have been used as the target for the structure-based drug discovery. However, it is challenging to find the selectivity of ATP binding site because they are highly conserved. In our previous studies, we presented the method for predicting the selectivity of the protein kinase inhibitors based on the water ring network analysis in the binding site. Here we tried to find a hit compound from in house database by targeting IRAK4. Using the selected hit compound, we explored the purchasable compounds known as inhibitor against the specific kinases, which have similar water ring network in binding site compared with IRAK4, and we carried out in vitro activity test for our target. Also the early hit compound was optimized using the structural information that we found from watering network analysis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-487**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of 3,4,5-trimethoxybenzene derivatives with substituted triazole group by Huisgen 1,3-cycloaddition and their inhibitory effects on 3T3-L1 adipocyte differentiation

오상태 김태정[1] 함정엽[1,*] 이석준[2,*]

가톨릭관동대학교 의과대학 기초과학교실 [1]한국과학기술연구원(KIST) 천연물연구소 [2]가톨릭관동대학교 의과대학 약리학교실

Combretastatin is a bisbenzylic stilbene natural product that was first isolated from the bark of Combretum caffrum, which is commonly known as South African Bush Willow. Among combretastatins, combretastatin A-1 (1) and A-4 (2) are potent anticancer agents that strongly inhibit tubulin polymerization by competing with colchicine (3), which have a 3,4,5-trimethoxybenzene group in their structures. It is supposed to be a critical role in the mechanism of action of the aforementioned drugs. To discover novel anticancer drug, we designed novel structure for a 3,4,5-trimethoxybenzene derivative (4) with variously substituted 1,2,3-triazole group groups, and named them as “combretastatin mimic library”. However, they are no or weak cytotoxic effect against three cancer cells, DLD-1, A172, and B16. To further investigate the biological properties of the synthetic combretastatin mimic library (5a – 5k), we conducted several bioassay. The results from the screenings we conducted indicated that the library (5a – 5k) showed a moderate to strong inhibitory effect against 3T3-L1 adipocyte differentiation. In this presentation, we will show that synthetic combretastatin mimic library effectively inhibited 3T3-L1 adipocyte differentiation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-488**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Biological Activity of α, β-unsaturated carbonyl conjugated carboxylic acid derivatives as S1P Receptor Agonist

황보희* 최영진[1,*] 서선희[2] 백두종 남길수[3,*]

상명대학교 화학과 [1]과학기술연합대학원대학교(UST) [2]한국과학기술연구원(KIST) 뇌의약연구단 [3]한국과학기술연구원(KIST) 뇌과학연구소

Multiple Sclerosis (MS) is an inflammatory and chronic disease of the central nervous system (CNS). MS is a demyelinating disease in which the insulating covers of nerve cells in the brain and spinal cord are damaged. This damage disrupts the ability of parts of the nervous system to communicate. In 2010, Novatis developed the first oral drug Fingolimod as a S1P receptor agonist. Fingolimod binds S1P1 receptor and effects as a functional antagonist. Initially, the ligand binds S1P receptor-1(S1P1R) and then leads internalization of S1P1R on T-cells. Down-regulation of S1P1R on lymph node T-cells renders lymphocytes unresponsive to the egressive signal and prevents infiltration of pathogenic T-cells into the CNS[1] . However, Fingolimod is a non-selective S1P1R and then induces several side effects such as bradycardia. We have found some active compounds against S1P1 from the Korean marine natural extracts. Among them, the most active compound W-137-6F5E showed ED50 = 8.2 • M. To develop potent and reduced side effective MS treatments, we tried to find selective S1P1 and S1P5 agonists. Based on the chemical structure of W-137-6F5E, we designed and synthesized of various α, β-unsaturated carbonyl conjugated carboxylic acid derivatives. In this poster, the detailed synthesis and their biological activity against S1P1 and S1P5 receptor are described. 1. Marc Bigaud , Danilo Guerini, Andreas Billich, Frederic Bassilana, Volker Brinkmann, Second generation S1P pathway modulators: Research strategies and clinical developments, Biochimica et Biophysica Acta 1841 (2014) 745–758

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-489**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Diversity-Oriented Synthetic Strategy for Developing a Chemical Modulator of Protein–Protein Interaction

김종훈 박승범[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Diversity-oriented synthesis (DOS) can provide a collection of diverse and complex drug-like small molecules, which is critical in the development of new chemical probes for biological research of undruggable targets. However, the design and synthesis of small-molecule libraries with improved biological relevance as well as maximized molecular diversity represents a key challenge. Herein, we employ functional group pairing strategy for the diversity-oriented synthesis of a chemical library containing privileged substructures, pyrimidodiazepine or pyrimidine moieties, as chemical navigators toward unexplored bioactive chemical space. To validate utility of this DOS library, we identify a new small-molecule inhibitor of LRS–RagD protein–protein interaction (PPI), which regulates the amino acid-dependent activation of mTORC1 signaling pathway. This work highlights that privileged substructure-based DOS (pDOS) strategy can be a powerful research tool for the construction of drug-like compounds to address challenging biological targets.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-490**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

development of dabigatran based imaging agent for blood clots

<u>문용</u> 최성욱*

충남대학교 신약개발학과

과도한 blood clot 의 생성은 인체내에 뇌졸증. 심장마비 등의 치명적인 결과를 유발한다. 보통 이러한 인체 내부의 과도한 blood clot 의 확인은 기계 장비를 통하여 이루어져 왔다.그러나 그러한 절차들은 매우 까다롭고 비용적인 부분도 부담이 되기 때문에 이러한 부분을 해결하고한다. 그러한 방법으로써 현재 혈액응고제로 쓰이고 있는 dabigatran 의 구조를 바탕으로 한 화학 물질을 합성하고 이 물질의 활성에 대해서 연구한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-491**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of Novel Indazole Analogs for CDK2 Inhibitors

Gangadhar Rao Mathi 황종연* 하재두[1,*] 김필호*

한국화학연구원 의약화학연구센터 [1]한국화학연구원 난치성질환치료제연구센터

Cyclin-dependent kinases (CDKs) are protein kinases involved in cell cycle regulation and mRNA synthesis and processing. Aberrant expression or dysregulation of CDKs has been implicated in the pathogenesis and progression of multiple human cancers. Overexpression of individual complexes are reported in multiple myeloma (MM), making them attractive therapeutic targets. AT7519 is a small molecule inhibitor of multiple cyclin-dependent kinases (CDKs) which shows encouraging anti-cancer activity against multiple cell lines and in tumor xenografts.Cyclin dependent kinase 2 (CDK2) is thought to be a crucial regulator of S-phase progression and is therefore evaluated as an anticancer drug target. Neuroblastomas are childhood tumors with an often lethal outcome. It has been known that about twenty percent of the tumors have MYCN amplification, and these tumors are ultimately refractory to any therapy. Targeted inhibition of CDK2 leads to induction of apoptosis in MYCN-amplified neuroblastoma cells. The synthetically lethal relationship between CDK2 and MYCN indicates that CDK2 inhibitors could be potential MYCN-selective cancer therapeutics.A new series of chemical entities were designed and synthesized based on the structure-guided optimization of indazole. The compounds prepared were tested for their inhibitory activities against CDK2 and CDK5 enzymes. The synthesis and structure-activity relationship of analogs prepared will be discussed.

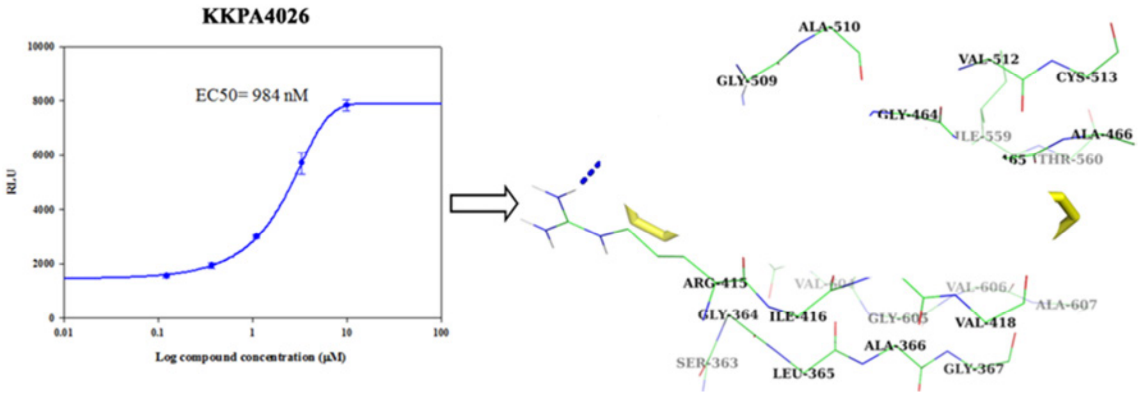
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-492**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

In Silico Identification of a Sulforaphane Superior Hit Compound and Its Scaffold-guided Synthesis of a Novel Class of Keap1-Nrf2 Modulators

박아영 배애님[1,*] 최기항

고려대학교 화학과 [1]한국과학기술연구원(KIST) 생체과학연구본부

Redox-sensitive kelch-like ECH-associated protein-1 (Keap1)-nuclear factor erythroid 2-related factor 2 (Nrf2) pathway has been explored as a sensible target to ameliorate oxidative stress-induced pathological responses by the transient activation of Nrf2. Present study has practiced a Keap1-targeted therapeutic intervention method for the non-covalent inhibition of Keap1-Nrf2. An integrated structure- and ligand-based design principles were applied to formulate feature-based pharmacophores that queried against the chemical databases. In vitro screening of the hits produced a potential compound, KKPA4026, superior to sulforaphane in terms of functional activity with an EC50 of 984 nM. This scaffold was further optimized by the docking of synthetically available analogs. These results led us to the design, synthesis, and biological evaluation of a novel class of Keap1-Nrf2 modulators.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-493**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and biological evaluation of ^{18}F labeled benzamide derivatives as a potential PET agent for malignant melanoma

표아영 김동연[1,*]

전남대학교 화학과 [1]화순전남대학교 병원

Malignant melanoma is a very aggressive and the most serious form of skin cancer. The incidence of this cancer has been increasing worldwide and there is still no effective treatment. Early detection in the earliest stages is very important to accomplish positive result and improve the survival of patients through therapy. In this study, we synthesized novel several kinds of ^{18}F labeled benzamide derivatives using N-succinimidyl 4-[^{18}F]fluorobenzoate ([^{18}F]SFB) as prosthetic group. Furthermore, we evaluated biological characteristics in B16F10 (mouse melanoma) tumor bearing mice and lung metastatic models. Reaction time of labeling was within 30 min at 60 ^{o}C and the overall non decay-corrected radiochemical yield was approximately 10–15%. We performed microPET studies with [^{18}]DMFB and B16F10 tumor was visible after injection of [^{18}F]DMFB immediately. [^{18}F]DMFB accumulated in tumor after i.v. injection and retained for whole time (over 60 min). In biodistribution studies, tumor uptake of [^{18}F]DMFB (10, 30, 60 and 120 min % ID/g: 12.51, 12.17, 10.89, 8.7) retained from 10 to 120 min. Liver uptake of [^{18}F]DMFB (10, 30, 60 and 120 min % ID/g: 20.76, 6.73, 3.0, 0.57) decreased from 10 to 120 min and showed fast clearance from liver. [18F]DMFB demonstrated specific uptake in B16F10 tumor bearing model and might have a potential to be utilized as a novel melanoma imaging agent for PET.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-494**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of Novel S1P3-Sparing S1P1 & S1P5 Receptor Agonists for Treatment of Multiple Sclerosis

김효진 손우승[1] 서선희[2] 임상민[2] 백두종 배애님[3,*] 정규성[1]

상명대학교 화학과 [1]연세대학교 화학과 [2]한국과학기술연구원(KIST) 뇌의약연구단 [3]한국과학기술연구원(KIST) 생체과학연구본부

Multiple sclerosis (MS) is a chronic, progressive autoimmune disease in the CNS. The non-selective Sphingosine-1-phosphate (S1P) receptor modulator, FTY720, binds to S1P1,3,4,5. It could cause diverse side effects such as bradycardia. Our rationale of developing novel S1P1 & S1P5 agonist is to be lower the circulating lymphocytes more efficiently by internalization of S1P1 on lymphocyte and to remyelinate by modulation of S1P5 on oligodendrocytes. We attempted to design S1P1 & S1P5 dual receptor agonists via in silico study based on already disclosed S1P1 & S1P5 agonist such as ASP4058, BAF312, etc. Novel S1P3-sparing S1P1 & S1P5 agonists were identified by Calcium Signaling Assay, β-arrestin assay and Receptor internalization assay. Furthermore, several compounds act as β-arrestin biased S1P1 agonist. We are optimizing to improve pharmacokinetic properties remaining S1P1 & S1P5 affinity and selectivity against S1P2 - S1P4.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-495**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The discovery of Dyrk1A inhibitor based on the water net-ligand similarity method

윤혜리 김보경 강남숙*

충남대학교 신약전문대학원

Dual-specificity tyrosine-regulated kinases (DYRKs) have been found to implicate in regulating cell growth and development. DYRKs family consists of Dyrk1A, Dyrk1B, Dyrk1C, Dyrk2, Dyrk3, Dyrk4A, and Dyrk4B. Overexpression of Dyrk1A, one of member of DYRKs family, has been reported as the promising target for the treatment of the neurological abnormalities. The natural products such as harmine, epigallocatechin gallate, quinalizarin and the synthetic products such as INDY, meriolins, variolin B, meridianins, and also multitarget kinase inhibitors such as TBB, TBI, DMAT, TID are discovered as inhibitors for Dyrk1A. We carried out QSAR and docking study for identifying the novel scaffold against Dyrk1A with in-house kinase focused library. Also, we analyzed the kinase ATP binding site similarity based on the water network analysis via MD simulation and found one kinase. We optimized the obtained hit compounds using the water network-ligand similarity method.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-496**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

QSAR approach of acute inhalation toxicity by vapour exposure

김선호 이병훈 이민지 이성광*

한남대학교 화학과

When various chemicals flowed during everyday life inflow in respiratory organ, It is a common that noxious information of the chemicals are unknown well. Although more than 40,000 types of chemicals used in-country already has been distributed until the present, and new substances have increased every year, registering most of those is acted without theirs toxicity information. Owing to bags of time used and deal of money, However, it is impossible for people to realistically investigate the noxious information about innumerable chemicals. In case of situation, Quantitative Structure-Activity Relationship(QSAR) studies can provide a useful tool for predicting the toxicities of untested chemicals. The most significant purpose of the this study is developing the Quantitative Structure-Activity Relationship(QSAR) models in order to predict an LC50 for acute toxicity on inhalation. Acute inhalation toxicity LC50 data (4 hours, rats) which had been determined using OECD test guideline 403 obtained from echemportal website. Molecular descriptors were calculated from molecular structure using PreADMET program. The data set was divided into training set(60%) and test set(40%) by using sphere exclusion method(SEM). 2D descriptors, 3D pharm-RDF descriptors based on chemical feature and radial distribution function and machine learning methods such as multiple linear regression(MLR) and support vector machine(SVM) were used to develop predictive QSAR model. The chance correlation and predictability of these method validated by y-scrambling method and external validation. The reliable prediction range will be set from applicability domain(AD) based k-NN method.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-497**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and biological evaluation of marine-derived benzoxazole natural product as anti-cancer agents

이윤서 김태정[1] 노태섭[2] 김경민[3] 전상일[4] 함정엽[1,*]

강릉원주대학교 해양자원육성학과 [1]한국과학기술연구원(KIST) 천연물연구소 [2]한국과학기술연구원(KIST) 강릉분원 천연물연구센터 [3]강릉원주대학교 화학신소재학과 [4]강릉원주대학교 화학과

Recently, natural products obtained from the nature exhibit a lot of biological activities and it sometimes become to the lead compound for drugs. For example, natural products and its derivatives such as taxol, vincristine, morphine and codeine are already used as anticancer drugs and anodynia, and so on. Especially, these natural products are suitable in terms of safety for human, therefore, drug development from natural products has received much attentions in the world. Focusing on new drug development, we have been continuing to synthesize pharmacophores of natural products including biological activities and further modifying them to functionalized derivatives. Also, to further enhance effective methods to find natural product derivatives, our research has applied to the concept of *Naturomimetic Approach* developed by our group. Biologically active pharmacophore of natural product is synthesized and efficient research to find further moiety is conducted through Pd-catalyzed carbon-carbon coupling reactions. In the poster presentation, we will introduce our recent research results in *Naturomimetic Approach* from marine-derived benzoxazole natural product as anti-cancer agents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-498**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Improved Anticancer and Renoprotective Effects of Temperature and Pressure Controlled Microwave (TPC-MW) processed Ginseng

최필주 김규선[1] 송봉근[1] 전상일[1] 강기성 함정엽[2,*]

가천대학교 글로벌캠퍼스 한의학과 [1]강릉원주대학교 화학과 [2]한국과학기술연구원(KIST) 천연물연구소

Ginsenosides, the unique constituents of Panax plants, are the biologically active components of ginseng. Several methods for increasing the biological activities of ginseng by conversion of ginsenosides using thermal processing have been developed by us and others. In this study, we demonstrated the efficient structural conversion of ginsenosides, which enhances the biologically activity of ginseng by temperature and pressure controlled microwave (TPC-MW) irradiationTo confirm the anticancer effect of TPC-MW ginseng, it was tested in 8 human cancer cell lines (cervical cancer HeLa, gastric cancer AGS, colon cancer HCT-116, lung cancer A549, liver cancer HepG2 cells, and prostate cancer DU145, LNCaP, PC-3). Antiproliferation results for 8 human cancer cell lines treated with ginseng extracts indicate that PC-3 cells treated with TPC-MW ginseng showed the highest activity. We also showed that TPC-MW ginseng also suppressed the growth of human prostate cancer cell and cervical cancer cell xenografts in athymic nude mice as an in vivo model.The LLC-PK1 cell damage by cisplatin was significantly decreased by treatment with TPC-MW ginseng and ginsenosides Rg3, Rg5, and Rk1. We found that ginsenosides Rg3, Rg5, and Rk1 generated during the heat treatment of ginseng ameliorate renal damage by regulating inflammation and apoptosis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-499**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Setup and validation of shake-flask procedures for the determination of solubility

전수빈 한미정[1] 강남숙*

충남대학교 신약전문대학원 [1]충남대학교 생물공학연구소

The measurement and optimization of physicochemical properties of drugs such as ionization, lipophilicity, permeability, and solubility are fundamental to successful new drug discovery. Especially, aqueous solubility is very important property for the interpretation for the delivery to and efficacy against the druggable target. There are many different approaches which can be used to determine a solubility based on the pH-metric method, having the limitation at lower and upper pH range. Here we present the well-optimized shake-flask procedure. It requires the appropriate selection of the volumes of solvents to employ. We set up the assay, including evaluation of quantification method, equilibrium times, DMSO concentrations, and buffer conditions. A comparison of the known thermodynamic solubility results to the shake-flask solubility assay results is also discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-500**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Tetrasubstituted benzene derivatives as Pim kinases inhibitors

강지희 **HONG VICTOR SUKBONG** 이진호*

계명대학교 화학과

The Pim kinases (Pim-1, Pim-2, and Pim-3) are proto-oncogenic serine/threonine kinases and regulate both apoptosis and cellular metabolism. Pim kinases are regulating a number of signaling pathways that are fundamental to tumorigenesis. Overexpression of pim kinases has been observed in a range of human hematopoietic malignancies, such as leukemias and lymphomas as well as in prostate cancers. As such, pim kinases are one of the attractive therapeutic targets for the development of anti-cancer agents. The present report describes the identification of pim kinase inhibitors with high potency. A novel series of 1,2,3,4-tetrasubstituted benzene derivatives were designed to interact with ε-amino group of Lys67, carboxylate group of Asp128 as well as backbone carbonyl group of Glu121 in ATP binding pocket of Pim-1 kinase. Synthesized compounds showed potent inhibitory activities against Pim kinase. The most potent compound exhibited IC50s of 0.046 μM for Pim-1, 0.069 μM for Pim-2 and 0.013 μM for Pim-3

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-501**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

1,3-Disubstituted benzene analogues as Pim kinase inhibitors

이아연 HONG VICTOR SUKBONG[1] 이진호[1,*]

계명대학교 유기화학전공/화학과 [1]계명대학교 화학과

Overexpression of Pim kinases have been implicated as oncogenic drivers in multiple tumors including lymphoma, leukemia, multiple myeloma, prostate and gastric cancer. Pim kinases (PIM-1, PIM-2, and PIM-3) are involved in many cellular phenomena such as transcription, translation, growth, survival and apoptosis resistance of cancer cell. Thus, Pim kinases are potential targets for therapeutic intervention in cancer. Herein, we describe the discovery of Pim kinases inhibitors with high potency. A novel series of 1,3-disubstituted benzene derivatives were designed to interact with • •amino group of Lys67 as well as carboxylate group of Asp128 in ATP binding pocket of Pim-1 kinase. Synthesized compounds showed potent inhibitory activities against Pim kinases. The most potent compound exhibited IC50s of 0.060μM for Pim-1 and 0.032μM for Pim-3.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-502**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

SYNTHESIS AND BIOLOGICAL EVALUATION OF PYRIMIDINE DERIVATIVES AS GPR119 AGONISTS

김효진 유민진[1] 정관영[2,*]

서강대학교 화학과 [1]과학기술연합대학원대학교(UST) 한국화학연구원/의약화학 [2]한국화학연구원 의약화학연구센터

Diabetes is a serious metabolic disorder that occurs when the pancreas does not produce enough insulin, or the body cannot effectively use existing insulin. Hyperglycemia (high blood glucose) can lead to various health consequences such as kidney damage, heart disease, stroke, nerve damage and blindness. Type 2 diabetes mellitus (T2DM, or noninsulin dependent), is the most common form of diabetes caused by insulin resistance, and loss of pancreatic ß-cell function and approximately 95% diabetic patients are suffering from type 2 diabetes. GPR119 is a member of the class A G protein-coupled receptor (GPCR) family, and it is highly expressed in pancreatic ß-cells and intestinal endocrine cells. Upon activation by its endogenous ligand, intracellular cAMP accumulates and adenylate cyclase activation enhances the effect of glucose-stimulated insulin secretion (GSIS) and GLP-1 release. Thus GPR119 represents a promising target for the treatment of type 2 diabetes and obesity owing to its ability to improve glucose homoeostasis while concurrently slowing gastric emptying, reducing food intake and promoting weight loss Endogenous ligands for GPR-119 have been identified including lysophosphatidylcholine (LPC) and oleoylethanolamide (OEA). When Sanofi-Aventis agreed to get the right of MBX-2982 from Metabolex (Cymabay Therapeutics) in 2010, which was a representative orally active GPR119 agonist. However, Sanofi-Aventis opted to terminate the deal in May 2011, has a loss of efficacy durig its clinical trial. We looked in deeply of MBX-2982 and substituted tetrazole moiety to five-membered heterocylic ring which increased the activity (five-fold potent) and metabolic stability. Also, we modified ethylpyrimidine side of MBX-2982 with polar linkers

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-503**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of privileged Thiazolodiazepinones

김다현 김주빈 김소희 이태호*

경북대학교 약학과

The 1,4-benzodiazepine scaffold is utilized a lot in medicinal chemistry. For example, diazepam well-known as a drug for anxiety treatment contains a 1,4-benzodiazepine. Also, a variety of benzodiazepine derivatives are reported they have many biological activities.These have shown activities as inhibition the proliferation of tumor cells, antitrypanosomal activity, γ-secretase inhibitor, histone deacetylase inhibitors (HDACi), the peptide hormone cholecystokinin (CCK) antagonist, anticancer agent and p53-HDM2 interaction antagonist. In addition, by acting on central nervous system as GABA receptor agonists, they could be applied to insomnia, trouble sleeping and convulsion. Thus, they serve as attractive scaffolds for combinatorial library construction via solution-phase synthesis. Herewith, we have tried to construct a small molecule library based thiazolodiazepinone via solution-phase parallel synthesis. The synthetic strategy includes directly amide bond formation of 2-aminothiazole with protected glycine. After the additional diverse moieties are introduced, nucleophillic substitution is achieved with various amine nucleophiles to give 2,4,6,8-tetrasubstituted-thiazolodiazepinone derivatives in good overall yield.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-504**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Amyloid beta aggregation inhibitor

신문관

충남대학교 신약개발학과

AD(Alzheimer's disease)는 퇴행성 신경질환이며 뇌의 신경 세포와 시냅스의 기능의 파괴로 발병된다.초기에는 기억력, 행동, 말하기 등의 인지 기능에 이상이오며 말기에는 경직, 보행이상 등의 신경학적 장애를 동반 그 후 평균 8 년 후에 사망에 이른다고 한다. AD 의 첫번째 이유는 A-beta 라는 작은 단백질이 과도하게 만들어져 뇌에 침착되면서 뇌 세포에 유해한영향을 준다는 가설 그리고 두번째로는 뇌세포의 골격유지에 중요한 역할을 하는 타우 단백질의 과인산화, 염증반응, 산화적 손상 등으로 뇌세포 손상에 기여하여 발병한다고 생각하고있다. 그래서 우리는 이 두가지 이유중에 첫번째 이유를 들어 A-beta 의 aggregation 을 억제 할수 있다고 생각하는 물질인 FMHT([N-2-[fluoropropyl]-2-(4'-(methylamino)phenyl)-6-hydroxybenzo-thiazole}]) 을 기반으로 우측 amin 쪽과 좌측 aldhyde 쪽을 clogP 값이 더 낮은 것으로 변환시켜 A-beta fibrillogenesis 에 더 좋은 inhibitor 로 작용할 꺼라 생각 하여 실험을 진행중에 있다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-505**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gambogic acid induced apoptic cell death in glioblatoma cells

이희수 이재욱[1,*]

강릉원주대학교 치의학과 [1]한국과학기술연구원(KIST) 치매DTC융합연구단

Glioblastoma mutilforme (GBM) is most common and aggressive malignant primary brain cancer. 1 Therefore, the effective treatments of glioma are still required. We previously screen natural product libraries and we identified that Gambogic acid is potent a compound to glioblastoma cells. We tested gambogic acid for anti-proliferative effects on T98G and U87MG glioblastoma cell line. Gambogic acid exhibited induced apoptosis in T98G glioblastoma cell in a dose dependent manner. Western blot analysis of incubated gambogic acid with T98G cell revealed that increased Bax and AIF expression, cytochrome c release, and cleavage of caspase-3, -8, -9, and PARP, while Bcl-2 expression was downregulated. Our results indicate that GA increases Bax- and AIF-associated apoptotic signaling in glioblastoma cells.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-506**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Renoprotective Chalcone Analogues That Protect Against Cisplatin-induced Cytotoxicity in LLC-PK1 Cells

이재욱* 이희수[1] 강기성[2,*]

한국과학기술연구원(KIST) 치매DTC융합연구단 [1]강릉원주대학교 치의학과 [2]가천대학교 글로벌캠퍼스 한의학과

Fifteen chalcone analogues were prepared and evaluated for renoprotective effects using cisplatin-treated cultured kidney cells (LLC-PK1). In particular, chalcone derivatives (14 and 15) with allyloxyphenyl and chloro substitution group show highly potency in renoprotective effects. In our further study using compound 15, blocking the MAPKs-caspase 3 signaling cascade plays an important role in mediating the protective effect of these chalcone derivatives against cytotoxicity in cultured LLC-PK1 cells.

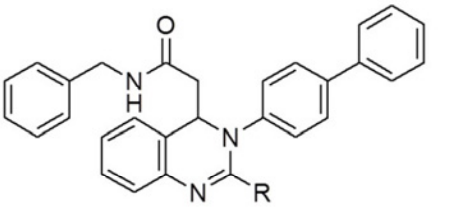
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-507**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

3,4-Dihydroquinazoline Derivatives as Selective Butyrylcholinesterase Inhibitors

김진한 박병연 남지혜 이재열*

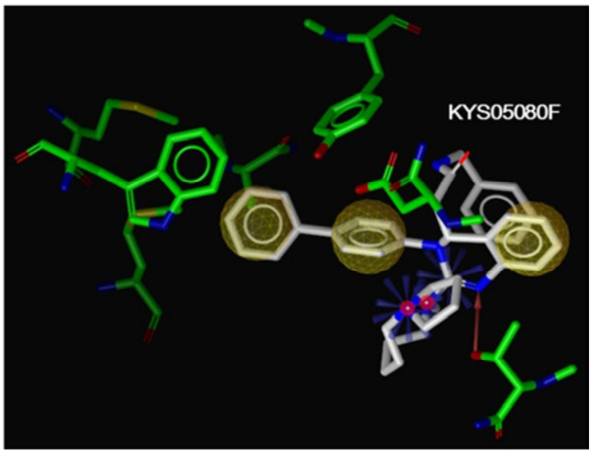
경희대학교 화학과

A series of 3,4-dihydroquinazoline derivatives were evaluated as cholinesterase inhibitors. The results showed that most of compounds could inhibit butyrylcholinesterase (BChE) with IC_{50} values ranging from 5.3 into 0.045 • M, with two of them moderately inhibiting also the acetylcholinesterase (AChE). In particular, KYS05080F and KYS05090S showed the most potent activity against BChE with IC_{50} values of 45 nM and 62 nM, as well as 146- and 161-fold higher affinity to BChE, respectively. Moreover, all compounds exhibited a weak or no inhibitory effect on amyloid-β (Aβ) (1-40) self-aggregation at 100 μM concentration. To understand the excellent activity of these compounds, molecular docking simulations were performed to get better insights into the mechanism of binding of 3,4-dihydroquinazoline derivatives. As expected KYS05080F and KYS05090S bind to both catalytic anionic site (CAS) and peripheral site (PS) of BChE with better interaction energy values than AChE, in agreement with our experimental data.



KYS05080F: R = $-N(CH_3)(CH_2)_5N(CH_2)_4$
IC_{50} = 45 nM against BChE; S.I. = 146

KYS05090S: R = $-N(CH_3)(CH_2)_5N(CH_3)_2 \cdot 2HCl$
IC_{50} = 62 nM against BChE; S.I. = 161



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-508**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of A2B corroles for the application of photodynamic therapy

윤새미 선경표 하용황[1,*]

중원대학교 의약화학과 [1]중원대학교 의약바이오학과

It is hard to remove individual tumor cells individually by surgical operations because they are too small to remove via naked eyes. Many researches have been interested in developing tumor-specific destruction method. As an alternative therapeutic skill, photodynamic therapy (PDT) attracts great interest due to its high selectivity. PDT is based on the photosensitizers which can generate singlet oxygen by energy transfer from triplet excited state sensitizer to molecular oxygen in ground state. Herein, we designed two types of A2B corroles as photosensitizers, synthesized, and characterized the photophysical properties via measuring of UV-vis absorbance, and emission spectra, etc. For the next step, we are planning to synthesize various halogenated metallocorroles and investigating phosphorescence properties and application for tumor removal potential in cellular level.

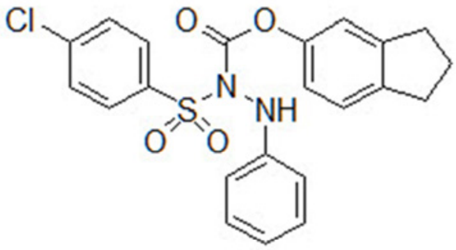
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-509**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis, structure determination, and biological evaluation of phenylsulfonyl hydrazide derivatives as potential anti-inflammatory agents

정희락 김광종 박은별 임지웅[1] 이재균[2] 이재열*

경희대학교 화학과 [1]경희대학교 융합과학기술학과 [2]한국과학기술연구원(KIST) 케모인포매틱스연구단

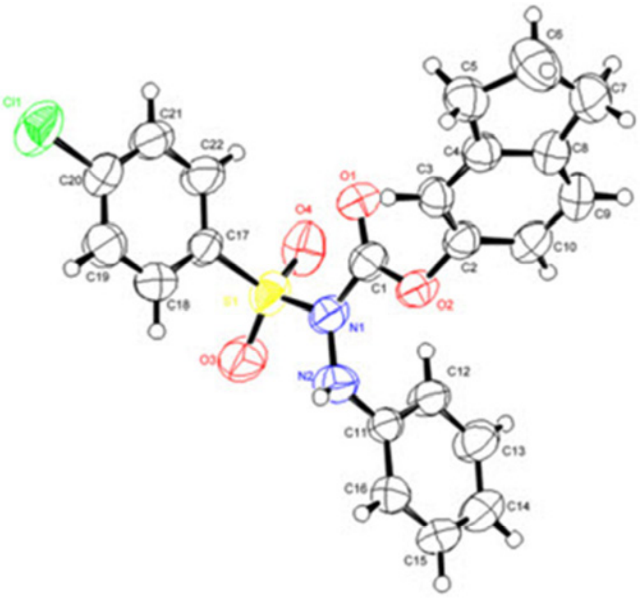
A novel series of phenylsulfonyl hydrazide derivatives were found to reduce LPS-induced PGE_2 levels in RAW 264.7 macrophage cells via an inhibition of mPGES-1 enzyme. Recently, it was found that a regioisomeric mixture of phenylsulfonyl hydrazide was formed depending on the reaction conditions, which favor either of two regioisomers. One regioisomer corresponds to a kinetic product (7a-7c) and the other regioisomer corresponds to a thermodynamic product (8a-8c). Among them, the structure of kinetic product 7b was confirmed by measuring single X-ray crystallography. In vitro PGE_2 assay studies showed that the kinetic product (7a and 7b; IC_{50} = 0.69 and 0.55 μM against PGE_2) is generally more potent than the thermodynamic product (8a and 8b; IC_{50} = > 10 and 0.79 μM against PGE_2). A molecular docking study also exhibited that the kinetic product (7a) has a higher MolDock Score (-147.4) than that of 8a (-142.4), which is consistent with the PGE_2 assay results. A new potent phenylsulfonyl hydrazide (7d; IC_{50} = 0.06 μM against PGE_2) without affecting COX-1 and COX-2 enzyme activities was identified based on these overall results.



7b

PGE$_2$: IC$_{50}$ = 0.55 μM

No activity against COX-1/2



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-510**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Identification of antioxidants and tyrosinase inhibitors from *Lespedeza cuneate* G. Don using off-line and ultrafiltration combined with HPLC

지준* 임순성[1]

에프에이 부설연구소 [1]한림대학교 식품영양학과

Lespedeza cuneate G. Don is one of plant species of leguminosae family widely distributed in eastern and southern Asia. It is used as traditional asian medicine for treatment of the diseases of the liver, kidneys and lungs. A previous study has reported that*L. cuneate* extract showed excellent antioxidant capacity and tyrosinase inhibitory activity. However, there is no research reports the antioxidants and tyrosinase inhibitors existed in *L. cuneate* even though its chemical constituents have been well analyzed. In the present study, The *L. cuneate* was extracted by 70% ethanol. In order to rapidly identify the antioxidants and tyrosinase inhibitors from *L. cuneate*, the off-line ABTS-HPLC assay and ultrafiltration-HPLC assay were performed. In results, vitexin, kaemferol, astragalin, and quercetin were identified as antioxidants, and vitexin was identified as the tyrosinase inhibitor from *L. cuneate*. These results suggest that the extract of *L. cuneate* has the potential use as antioxidants and skin whitening agent, and off-line ABTS-HPLC and ultrafiltration-HPLC could be useful for high-throughput identification of antioxidants and tyrosinase inhibitors in natural products.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-511**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Hydration Pattern Analysis in the Crystalized Protein Structures

최광은 김만선 강남숙*

충남대학교 신약전문대학원

To investigate the hydration effect playing an important role in the function and structures of biomolecules, we analyzed the released crystal structures of proteins containing water molecules, which have effects on functions, a catalytic activity, and solubility of the protein. Protein structures showing low resolution (> 2.5 Å) were excluded, and then the distance between water and atoms in protein was calculated (r< 3.2 Å). Also we analyzed the patterns of water distribution; the frequencies and shapes in water network nearby the binding sites ranging from 5 Å to 6.5 Å around ligand. We identified that polar residues (Glu, Asp, Arg, Lys) have more interaction numbers than nonpolar residues (Gly, Ala) with water molecules. In case of residues containing large molecule weight (Phe, Trp, Met, Cys), interaction numbers with water molecules were the smallest. Furthermore, we analyzed water network around ligand binding site

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-512**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of Novel Antiviral Compounds Against Human Rhinovirus Infection

김진우 이주연[1] 한수봉[2] 정영식[3,*]

한국화학연구원 의약화학연구센터 [1]한국화학연구원 한국화합물은행 [2]한국화학연구원 신약연구본부 [3]한국화학연구원 신물질연구단

Enterovirus, which belongs to genus *picornaviradae*, has caused various diseases on mammalian species. Among those, human rhinoviruses (hRVs) have been concerned as the caustic agent for common colds as well as exacerbation of asthma and chronic obstructive pulmonary disease (COPD). Despite of continuous efforts for the treatment of hRVs, its high diversity had retarded the development of anti-hRV agents. Recently, we have developed a series of anti-hRV compounds which showed two-digit nanomolar reactivity with significant selectivity indices (>200) against both hRV-A and hRV-B strains. Time-of-addition study suggested that the novel compounds act at early stage of the viral invasion, while the resistant mutation was found in VP3-L25. Molecular docking simulation suggested their binding into VP1 capsid canyon, having significant interaction with VP3 side chain. Moreover, the novel compounds also showed remarkable reactivity against poliovirus 3 (PV3), implying their potential effectiveness against other picornavirus species.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-513**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Antiviral Activity of N,N' Disubstituted Ureas and Thioureas of p-benzene sulfonamide derivatives against Human Rhinovirus

chakarasali prashant Yashwardhan Malpani[1] 한수봉[2,*] 정영식[3,*]

과학기술연합대학원대학교(UST) Medicinal&Pharmacentical chemistry [1]과학기술연합대학원대학교(UST) 의약 약품화학 [2]한국화학연구원 신약연구본부 [3]한국화학연구원 신물질연구단

A series of disubstituted urea and thiourea derivatives of p-benzene sulfonamide were prepared containing one or two methylene group/s as linker between them. The compounds were synthesized in very simple and convenient synthetic route. These were tested for their inhibition property against HRV-A and HRV-B. In particular, the prepared compounds were tested against three different strains of Human Rhinovirus viz., HRV14, HRV21 and HRV 71. Some of the compounds synthesized have sub-micro molar range of activity against HRV 21 and HRV 71 and moderate activity against HRV 14. Also, these have overall a low cytotoxicity and thus high selectivity index values. Initial time of addition experiments shows that these compounds have quite similar mode of actions as *Pleconaril*, a capsid binding inhibitor.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MEDI.P-514**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

6,7,8,9-tetrahydrobenzo[4,5]thieno[3,2-*e*][1,2,4]triazolo [4,3-*a*]pyrimidin-5(4*H*)-one analogs with Polio, Coxsackie and Rhino Virus Inhibition Activity

BISWAS BISHYAJIT KUMAR Yashwardhan Malpani[1] 이상호[2] 한수봉[3] 정영식[4,*]

과학기술연합대학원대학교(UST) 의약 및 약품화학 [1]과학기술연합대학원대학교(UST) 의약 약품화학 [2]한국화학연구원 신약연구단 [3]한국화학연구원 신약연구본부 [4]한국화학연구원 신물질연구단

A series of 6,7,8,9-tetrahydrobenzo[4,5]thieno[3,2-*e*]triazolo[4,3-*a*]pyrimidin-5(4*H*)-one analogs (A), were synthesized and tested for their inhibitory activity against representative picornaviruses. A brief structure activity relationship (SAR) could be established with activities in micro-molar range for the best compounds. The prepared compounds were tested against Coxsackie B1 (Cox B1), Coxsackie B3 (Cox B3), Poliovirus 3 (PV3), Human Rhinovirus 14 (HRV14), Human Rhinovirus 21 (HRV21) and Human Rhinovirus 71 (HRV71). Some of these compounds showed good activity (selective index values >10) against these representative picornaviruses. The presence of tert-butyl side chain on the fused tetrahydrobenzene ring was highly essential for the activity of these analogs against these picornaviruses. Initial time of addition study rules out capsid binding inhibition at entry stages but it is expected to act at later stage/s of picornavirus lifecycle/replication. The present study resulted in discovery of triazolothienopyrimidinones as novel skeleton against picornaviruses.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-448**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly symmetric 26-facets rhombicuboctahedron and 50-facets polyhedron Cu_2O microcrystals

여별이 허영덕*

단국대학교 화학과

Various morphologies of Cu_2O microcrystals including cube, beveled cube, 26-facets rhombicuboctahedron, and highly symmetric 50-facets polyhedron were synthesized by reduction of copper ions by D-(+)-glucose with NaOH. The morphological evolution form cube, through beveled cube and 26-facets rhombicuboctahedron, to 50-facets polyhedron was observed with increasing the reactant NaOH concentration by selective adsorption of hydroxide (OH^-) ions to the positively charged on {110} and {111} facets. The simultaneous crystal growth along the {110} and {111} facets from the cube covered by only {100} facets produced the edge- and corner- truncated cube, that is beveled cube, and rhombicuboctahedron. Further increasing the NaOH concentration, the high-index {522} facets are grown to form the highly symmetric 50-facets polyhedron.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-449**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

An effective route for the room temperature formation of Pd-coatings on multiwalled carbon nanotubes in aqueous solutions

송재희

순천대학교 화학과

We present an easy one-pot synthesis route for the production of palladium nanoparticles and multiwalled carbon nanotubes (MWCNTs)-supported Pd-nanomaterial composites by a simple proton beam irradiation process in an aqueous solution at room temperature. Pristine and surface-modified MWCNTs were used to prepare MWCNT-Pd hybrids. Pd nanoparticles on the surfaces of MWCNTs were produced in situ in an aqueous solution without the addition of any harsh reducing agent. Pristine and thiolated MWCNTs were both densely decorated with spherical Pd nanoparticles and eventually Pd nanowire formation on MWCNTs was realized when reaction times exceeded 60 min. The thicknesses of Pd coatings on MWCNT surfaces were controlled by varying the concentration of MWCNTs in the reaction mixture. MWCNT-Pd composites were characterized by time-resolved transmission electron microscopy (TEM), selected area electron diffraction (SAED), and energy dispersive X-ray spectroscopy (EDS), and the results obtained revealed that Pd coatings were continuous, and resulted in a MWCNT-supported Pd nanowire structure.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-450**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Room Temperature Preparation of Pt-Decorated MWCNTs by Using Proton Beam Irradiation

<u>송재희</u>

순천대학교 화학과

We present a facile one-pot preparation route for the production of multiwalled carbon nanotube (MWCNT)-Pt nanoparticle composites in an aqueous solution at room temperature by using proton beam irradiation process without the addition of any reducing reagents. We utilized hexadecyltrimethylammonium bromide (CTAB)-stabilized pristine and thiol-functionalized MWCNTs for the synthesis of MWCNT-Pt nanoparticle composites and compared the deposition trends of the platinum nanoparticles onto the surfaces of pristine MWCNTs and surface-modified MWCNTs, respectively. Thiolated MWCNTs were densely and uniformly decorated with Pt nanoparticles while pristine MWCNTs were not. The Pt nanostructures on the surfaces of MWCNTs were spherical, and the average diameter was in the range of ~2 nm. Also, two different metal precursors, H2PtCl6 and Na2PtCl6, were used to find any distinguishable decoration patterns on the surface-modified MWCNTs; however, the deposition patterns were observed to be not very different.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

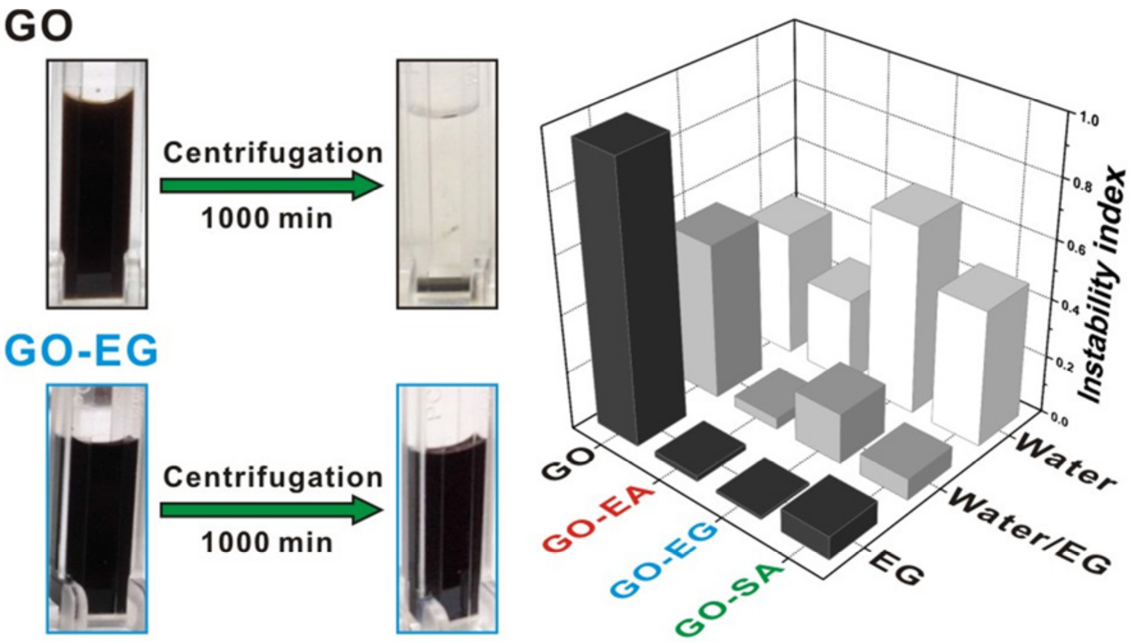
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-451**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Tailoring Graphene Nanosheets for Highly Improved Dispersion Stability and Quantitative Assessment in Non-Aqueous Solvent

박민주 김병수[1,*]

UNIST 에너지공학부 [1]UNIST 화학과

Aggregation is a critical limitation for the practical application of graphene-based materials. Herein, we report that graphene oxide (GO) nanosheets chemically modified with ethanolamine (EA), ethylene glycol (EG), and sulfanilic acid (SA) demonstrate superior dispersion stability in organic solvents, specifically EG, based on the differences in their covalent chemistries. Functionalized GO was successfully dispersed in EG at a concentration of 9.0 mg mL^{-1} (0.50 vol%), the highest dispersion concentration reported to date. Moreover, our study introduces a unique analytical method for the assessment of dispersion stability and successfully quantifies the instability index based on transmission profiles under centrifugation cycles. Interestingly, GO-EG and GO-EA exhibited highly improved dispersion stabilities approximately 96 and 48 times greater than that of GO in EG solvent, respectively. This finding highlights the critical role of surface functional groups in the enhancement of chemical affinity and miscibility in the surrounding media. We anticipate that the novel structural designs and unique tools presented in this study will further the understanding and application of chemically functionalized carbon materials.


GO
Centrifugation
1000 min
GO-EG
Centrifugation
1000 min
1.0
0.8
0.6
0.4
0.2
0.0
Instability index
GO
GO-EA
GO-EG
GO-SA
Water
Water/EG
EG

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-452**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One step synthesis of gold nanorods(NRs) using β-diketoamide

김곤희 송재희[1,*]

순천대학교 기초의.화학부 [1]순천대학교 화학과

Nanoscale materials have different characteristics from the bulk materials, such as optical, electronic, magnetic, and catalytic properties. That is why it has been an essential subject in basic science research as well as in technological applications. These properties are strongly depended on the size and shape of the particle, so it is very important to finely control the morphology of the nanomaterials. The synthesis and characterization of gold nanorods(NRs) have been carried out by reduction of the gold salt, HAuCl4. This has been done using a single reducing agent, such as β-diketoamide. We were able to synthesize gold nanorods in various conditions at room temperature which were found to greatly affect both the rate at which the nanorods form and their physical dimensions. The concentrations of reducing agents and silver nitrate used relative to the gold salt were found to alter the aspect ratio of the nanorods formed. Nanorods formed under optimum conditions were investigated using TEM.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-453**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Surfactant-Assisted Shape Evolution of 3D Molecular Architecture

<u>전묘빈</u> 권선범[1] 이희승[*]

KAIST 화학과 [1]Institut Européen de Chimie et Biologie 2, Rue Robert Escarpit 33607 Pessac Cedex, France.

Rational design of three-dimensional (3D) organic materials has made some progress, but it is still in its infancy. A class of self-assembly of artificial biomolecules using surfactants is presented that form nano/microscale supramolecular 3D materials in aqueous media. Here, we demonstrate the role of ionic surfactant cetyltrimethyl ammonium bromide (CTAB) in shape evolution of 3D molecular architectures (foldecture) obtained from the self-assembly of a • •peptide foldamer. Moreover, molecular dynamics simulation provided a reasonable explanation for the formation of 3D molecular architectures and interactions between surfactants and building block peptides in detail.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-454**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Photo-degradation of Ir complex in OLED device

배소현 강주연 손정배 김경우[1] 권장혁[1] 김성근[*]

서울대학교 화학부 [1]경희대학교 정보디스플레이학과

Extended operation of organic light-emitting diodes (OLEDs) results in materials degradation. To investigate the degradation mechanism of an iridium doped OLED device, we introduced photo-induced degradation to mimic the operational damage of OLEDs. We observed a loss of photoluminescence after light irradiation, and found that the intensity loss was dependent on the irradiation wavelength. Considering that the triplet metal-centered orbital (3MC) is related to the degradation of the Ir complex, we suggest that the wavelength-dependent optical transition governs the population of the 3MC state and the degradation of OLED. Our result suggests that Ir complex should be vulnerable to the short wavelength emission from the device, particularly from white OLED that emits over a broad range of wavelengths.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-455**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of polaron trap on degradation of OLED

강주연 배소현 손정배 김경우[1] 권장혁[1] 김성근[*]

서울대학교 화학부 [1]경희대학교 정보디스플레이학과

Despite the vital importance of understanding the underlying cause and the detailed mechanism of the degradation of organic light-emitting diodes (OLEDs) to improve the device stability and performance, much is hitherto unknown. We carried out transient electroluminescence (TREL) experiments to elucidate the effect of polaron traps on OLED degradation. We found that OLED materials develop polaron traps in the device and the number of such traps increases as the device becomes degraded. Using the definition of delay time as the time between the first application of operating voltage to the OLED device and the light emission, we found that the delay time decreases as the device undergoes degradation. It means that there exist polarons in the device that encounter each other earlier than polarons freshly generated from the electrodes by the operating voltage, which suggests that they must have been generated in the preceding cycle of OLED operation and remained in the trap when the OLED operation was stopped.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-456**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

CO_2 absorption mechanism of A_2CO_3 (A=Li, Na, K)-promoted MgO

곽진수 김강영 오경렬 권영욱*

성균관대학교 화학과

CO_2 capture and sequestration (CCS) is regarded as a key technology to reduce the concentration of CO_2 generated by large anthropogenic point source. CCS technology involves capture, transport and sequestration of CO_2. In capture process, post-combustion technology appears to be the most feasible at present because its implementation requires least cost. CO_2 absorbents for the post-combustion process are divided into three types depending on the operating temperatures; low (-200 ^oC), intermediate (200-500 ^oC) and high (above 500 ^oC). Currently, materials based on MgO are widely investigated for intermediate temperature absorbents.Magnesium carbonate ($MgCO_3$) decomposes into oxide at the lower temperature among all of the alkali and alkaline earth metal carbonates. In addition, the theoretical absorption capacity of MgO (for the reaction $MgO + CO_2 \rightarrow MgCO_3$) is the highest among all of the absorbents investigated so far. However, very large lattice energy of MgO originating from the large charge density of Mg^{2+} makes both absorption and desorption kinetics slowly. In order to enhance the absorption and desorption properties of MgO, A_2CO_3 (A=Li, Na, K)-promoted MgO is investigated as a CO_2 absorbent material. Our study indicates that CO_2 absorption occurs through formation of double carbonate (i.e., $MgO + A_2CO_3$ (A=Na, Li, K) $+ CO_2 \rightarrow A_2Mg(CO_3)_2$) and desorption through reverse reaction. The reaction kinetics of this absorbent is faster than that of MgO.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-457**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

$Ce(OH)_2Cl$ Film for Ce^{4+}/Ce^{3+} Redox-Controlled Luminescence 'Off/On' Switching

김민희 변송호*

경희대학교 응용화학과

$Ce(OH)_2Cl$ films were deposited on common quartz glass and FTO glass using hexamethylenetetramine (HMTA) in aqueous cerium chloride solutions at ambient pressure. XRD patterns of prepared films displayed quite different *(hkl)* intensity patterns depending on the substrate. Furthermore, the surface morphologies of $Ce(OH)_2Cl$ films deposited on common quartz glass and FTO glass substrates exhibited a clear difference in orientation. Coupled with complete disappearance of *(h0l)* reflections in XRD pattern, SEM images supported that the b-axis orientation is highly preferred in the film on FTO glass. Although both films showed similar blue emission intensity before oxidation, but the 'turn-off' efficiency by the oxidation reaction was much higher for the film on FTO glass. The effective blue 'turn-on' process was then achieved by the control of the Ce^{4+}/Ce^{3+} redox couple in an aqueous ascorbic acid solution. The reversible off and on switching of the $Ce(OH)_2Cl$ film was successfully operated without a significant degradation of the luminescence intensity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-458**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Removal and detection of Cu^{2+} ions in water by Eu-doped YVO_4-tailored LYH films

김현섭 변송호*

경희대학교 응용화학과

Copper is one of the essential metallic elements that our body needs. It is required for normal metabolic processes. However, too much intake of Cu^{2+} can lead to adverse health effects such as vomiting, diarrhea, stomach cramps, and nausea. It has also been associated with liver damage and kidney disease. The World Health Organization (WHO) and most of environment protection agencies limit the Cu content of drinking water to 31.5μM. Thus, detection and removal of such metal ions is of great importance. As YVO_4:Eu can be easily prepared, its high affinity toward Cu^{2+} ions could be exploited as an alternative method for copper detection. In this study, Eu-doped LYH films were coated on glass substrate by chemical bath deposition (CBD). These films were tailored with YVO_4 nanoparticles, which is also Eu-doped, when reacted with $NaVO_4$. As expected, the films showed strong red emission. When in contact with Cu^{2+} ions in water, however, it was observed that the emission intensity decreased. Due to the negative surface potential, the electrostatic attraction caused an intensive adsorption reaction of YVO_4:Eu nanoparticles with metal cations. The distinct fluorescence quenching of YVO_4:Eu was induced in the presence of Cu^{2+} ions. It is proposed that the complementary overlap of the emission band of YVO_4:Eu with the absorption band of Cu^{2+} results in the effective filter effect to quench the red emission. This new innovative approach can not only be used in the removal and detection of Cu^{2+} ions in water but can also be adopted to monitor the copper content as LYH films can be deposited on glass walls, containers, or tubes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-459**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Controlled Morphogenesis of Trigonal Pyramidal Carbamates at the Air Interface of Aminosiloxane-based Nanomatrixes

정의덕 이주윤[1,*]

한국기초과학지원연구원 하이테크소재연구부 [1]한국교통대학교 교양학부 - 화학

We present an unique mineralization process for the growth of trigonal pyramidal carbamates matrix-mediated from mesoporous KOH-catalyzed poly(γ-aminopropyl triethoxysilane) (PAPS), where CO_2 (0.03% v/v) from air is utilized as a carbon source and primary amine functionality of PAPS serves as an adhesive promoter for the aggregation of CO2$_2$(aq) and K+^{2} ions under relative humidity 50% ~ 60% at ambient temperature. The results from EDS, XRD, XPS, and Raman microscopy indicate that hydrogen-bonded cis-form of dimeric carbamate potassium salts is a primary constituent of the crystalline trigonal pyramids. The proposed mechanism would give rise to a catalytic crystallization strategy for producing hierarchically structured materials. This was supported by Korea National University of Transportation in 2016.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-460**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Sythesis and characterization of red organic phosphor for hybrid LED

이승민 정연태[1,*]

부경대학교 led융합공학 [1]부경대학교 융합디스플레이공학과

Solubility, thermal stability and luminous efficiency are main characteristics of organic phosphor for hybrid LED. Even though perylene bisimide derivatives have excellent thermal stability and luminous efficiency, they have low solubility in organic solvents. In this research, modified perylene bisimide derivative, N,N`-Bis(4-bromo-2,6-diisopropylphenyl)-1,6,7,12-tetraphenoxyperylene-3,4,9,10-tetracarboxyl bisimide (1), with phenoxy substituents at the bay positions of perylene and bromine atom in the benzene ring of imide was synthesized as an organic red phosphor. And (1) was characterized as a red organic phosphor for hybrid LED. The absorption and emission of (1) was shown at 576 nm and 610 nm in UV/Vis spectrum. In TGA thermogram, (1) showed good thermal stability without significant weight loss to 220 ℃. And in the solubility analysis, (1) showed the solubility of ≥ 3 wt% in general organic solvents.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-461**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect on the Geometric Structure of Additives for Stabilization of Liquid Crystalline-Blue Phases

이지혜 정 현*

동국대학교 화학과

We study on the stabilization of liquid crystalline-blue phases (BPs) depend upon the geometric structure of additives (linear and tetrahedral shape). BPs were classified the particular three phases as blue phase I (BPI), blue phase II (BPII) and blue phase III (BPIII) according to the alignment of double twist cylinders. BP I, II and III possess their different structure of disclination line as linear, tetrahedral and amorphous, respectively, which leads to narrow temperature range (normally less than 1.0 oC) due to the free energy cost of them as defect. Therefore, we introduce the two appropriate additives with linear and tetrahedral shape, cobalt oleate complex (Co-OL) and tetraoctadecylammonium bromide (TODAB), into the liquid crystal (mixture of 4-cyano-4'-pentylbiphenyl, JC-1041XX and chiral dopant) to stabilization of BP I and BP II, respectively. To demonstrate the stabilizing effect by introduction of additives, the temperature range of BPs is systematically investigate depending upon the geometric type and the addition amount of additives. From the results, the Co-OL introduced sample shows expansion of BP I range, and the TODAB introduced one indicates widening of BP II range due to the stabilization of each disclination line by introduction of suitable geometric structured additives.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-462**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Intense Solid-state Blue Emission of 9,10-Diphenylanthracene Incorporated in Mesostructured Materials

김아란 정 현*

동국대학교 화학과

The fluorescent mesostructured silica hybrid was obtained by in-situ synthetic route with 9, 10-diphenylanthracene (DPA) and tetraethoxysilane (TEOS) in the presence of a template surfactant amphiphilic triblock copolymer (P123). The structure and morphology of resulting hybrid have been characterized by powder X-ray diffraction (XRD), field emission scanning electron microscope (FE-SEM) and transmission electron microscope (TEM). The DPA molecules are successfully incorporated in mesostructured silica retaining a well-ordered hexagonal structure. Interestingly, the absorption and steady-state fluorescence spectroscopy reveal that the maximum peak of DPA is blue shifted after hybridization. The incorporation of DPA in mesostructured silica enabled to achieve high quantum yield. In fluorescence decay behavior of hybrid, high lifetime with low non-radiative decay is due to a reduced intermolecular interaction and a restricted intramolecular motion. The LED chip fabricated by hybrid show an outstanding blue color purity of LED chip with $CIE_{x,y}$ coordinates of (0.15, 0.03). Therefore, the fluorescent hybrid is considered a promising candidate for efficient deep-blue emitter in solid state.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-463**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile size controlled synthesis of fucoidan coated gold nanoparticles and cooperative anticancer effect with doxorubicin

장홍제

광운대학교 화학과

To conquer cancer, one of the most dangerous and common diseases faced by humanity, many therapeutic approaches have been researched and developed. Among them, discovery of highly effective therapeutic molecules without side effects and novel strategies for their effective delivery are the areas receiving recent global interest. Here, we accomplished the facile synthetic method for gold nanoparticles which surface coated with promising anticancer biopolymer, fucoidan (extracted natural product from brown seaweed) by one-pot manner for enhancing therapeutic and delivering efficacy with well controlled size distribution. Moreover, stable surface modification of fucoidan coating followed by conjugation of doxorubicin through cleavable linkage, significantly improve the anticancer effect of them. Present gold nanoparticles with doxorubicin conjugated fucoidan coating exhibited greatly enhanced anticancer effect than any other related platforms consisted with fucoidan based cancer treatment by adopting the nanoparticle integrated system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-464**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile large-scale synthesis of zeolite-templated microporous carbons with fully graphene-like frameworks through calcium-catalyzed ethylene carbonization

김경수 권용현[1] 이태경[1] 유 룡[2,*]

기초과학연구원 나노물질및 화학반응 연구단 [1]KAIST 화학과 [2]기초과학연구원 나노물질및화학반응연구단

Very recently, our group has developed a zeolite-templated synthesis route to microporous 3D graphene-like carbons via lanthanum-catalyzed carbonization of ethylene. In the present work, instead of lanthanum, inexpensive calcium was studied as a catalyst for ethylene carbonization in a zeolite template in order to optimize the carbon synthesis, specifically for the large scale production. The synthesis using a calcium catalyst gave a high carbon yield based on the template pore volume, and exhibited no significant amount of carbon deposition on external surfaces (i.e., highly selective carbon deposition inside zeolite micropores). Resultantly, ordered microporous structures of zeolite X could be faithfully replicated into the carbon. Single crystal X-ray diffraction analysis indicated that the carbon had 3D graphene- or nanotube-like frameworks along the surface of zeolite pore walls, similar to the case of lanthanum catalyst. With a 70-g batch of carbon synthesis, we demonstrated the potential of this synthesis route for large-scale production that would bring about a wide range of practical applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-465**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of Cu_2XSnS_4(X=Zn, Fe, Mn, Ni) and their photocatalytic activity

박용광 정동운*

원광대학교 화학과

CuO, ZnO 와 SnO 를 2-methoxyethanol, thioglycolic acid 와 2-aminoethanol 에 분산시켜 $Cu2ZnSnS_4$ 를 제조하였다. Cu_2ZnSnS_4 가 충분히 성장하도록 용액을 일정 온도에서 방치한 후 300℃에서 열처리 하였다. 같은 방법으로 ZnO 대신에 FeO, MnO, NiO 를 이용하여 Cu_2XSnS_4(X=Zn, Fe, Mn, Ni)를 각각 제조하였다. 얻어진 화합물들은 가시광선 영역에서 흡광이 발생하였다. Cu_2XSnS_4(X=Zn, Fe, Mn, Ni)화합물들은 P-25 에 비하여 가시광선 영역에서 뛰어난 촉매활성을 나타냈으며 Cu_2NiSnS_4, Cu_2MnSnS_4, Cu_2FeSnS_4, Cu_2ZnSnS_4 순으로 광촉매 활성이 증가하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-466**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

One-pot Synthesis of Boron and Sulfur co-doped Graphene Quantum Dots

기은별 김성진[1,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학과

Graphene quantum dots(GQDs) have attracted new interests due to their unique properties such as low cytotoxicity, chemical inertness, and stable photoluminescence in biomedical applications. There were reports that doping on GQDs with sulfur or nitrogen could improve their photoluminescence. Also, it has been suggested that heteroatom doping on GQDs could affect their chemical activities as well as rich luminescence properties on GQDs. Boron and sulfur co-doped GQDs could be obtained by one-pot hydrothermal treatment using a precursor consisted of boron and thiophene group. Since the defect of edge on GQDs can affect wavelength or intensity of PL, we used hydrogen peroxide in hydrothermal reaction. The GQDs characterized by TEM, EDS, XPS. UV-vis absorption and their fluorescence spectra were also investigated. Stable blue and green luminescence are observed on the boron and sulfur co-doped GQDs.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-467**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ternary Bulk Heterojunction of Nanostructured Perovskite-Low Bandgap Polymer-PCBM for Improved Efficiency of Organic Solar Cells

정한빈 이재관[1,*]

조선대학교 탄소소재학과 [1]조선대학교 화학교육과/탄소소재학과

Significant research efforts over the past years have been directed at developing efficient approaches such as developments of high-performance semiconducting materials such as low-band gap-conjugated polymer donors and fullerene derivative acceptors, effective functions with surface plasmon resonancing, charge transporting, optical spacing, and buffering in device structures, and morphological engineering of photosensitive films by post heat treatment, drying condition of casting solutions, or processing additives in an effort to improve the performance of solution-processed bulk heterojunction (BHJ) organic solar cells (OSCs) with a near-term goal of achieving a power conversion efficiency (PCE) above 10 %. Competitively this, solution-processable organometal halide perovskite solar cells have recently received considerable attention in the scientific community due to their promising breakthrough of over 15% PCE. In this work, we have developed a new organic-inorganic ternary bulk heterojunction (TBHJ) hybrid configuration comprised of nanostructured $(CH_3)_3NH_3PbI_3$ ($MAPbI_3$) perovskite, low bandgap polymer such as PCPDTBT, and PCBM for the hybrid devices of BHJ OSCs and perovskite solar cells. Well-organized BTJ films were readily prepared from sequential spin-casting of sparsely covered $MAPbI_3$ nano dots and PCPDTBT-PCBM BHJ composite on the ITO/PEDOT:PSS substrate. The outstanding performances were achieved from TBHJ hybrid devices configuration of ITO/PEDOT:PSS/$MAPbI_3$-PCPDTBT-PCBM/Al fabricated from BHJ system with DIO additive, which played a key role for developing perovskite structures of $MAPbI_3$ nano dots and induced the (110) directional crystallinity growth of the longitudinal constructive molphologies such as nano rods. The improved photocurrent and fill factor compared to those of conventional BHJ devices led to an increase in efficiency of ~28%. This improved photovoltaic performance originated from the higher quantum efficiencies contributed by the charge transfer from nanostructured $MAPbI_3$ perovskite to PCBM. These TBHJs composed of nanostructured $MAPbI_3$ perovskite, PCPDTBT, and PCBM also facilitated the exciton dissociation in the multi-BHJ system between $MAPbI_3$ perovskite, PCPDTBT, and PCBM.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-468**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly Efficient, Reproducible, Uniform$(CH_3NH_3)PbI_3$ Layer by Processing Additive Dripping for Solution-Processed Planar Heterojunction Perovskite Solar Cells

정한빈 이재관[1,*]

조선대학교 탄소소재학과 [1]조선대학교 화학교육과/탄소소재학과

Recently, solution-processable organometal halide planar heterojunction perovskite solar cells (PHJ PrSCs) have been of great interest. Because of their facile and inexpensive manufacturing processes, including versatile methods such as inkjet, doctor-blade, and roll-to-roll printing. As in particular, because the crystallinity, uniformity, and coverage of perovskite materials on the substrate are critical to improving the power conversion efficiency (PCE) of devices. Among them, solvent-engineering in which a solvent such as toluene, chlorobenzene, or ether is dripped briefly during casting of the perovskite precursor significantly improved crystallinity, uniformity, and coverage of perovskite materials. Also, incorporating a small amount of a processing additive such as dihaloalkane, chloronaphthalene, or ammonium halide into the perovskite precursor solution induced high crystallinity and a better morphology. However, the PHJ PrSCs were often fabricated with a small active area and still suffer from a large variation in device performance because the perovskite crystal grains were randomly formed in the solution-processed films. In addition several reports presented diiodooctane (DIO) played a key role in developing perovskite crystallinity, and the additive reportedly helped to form a smooth and uniform film with flawless perovskite nanocrystals.In this work, we attempted to induce a more uniform morphology in perovskite films by using the processing additive dripping (PAD) approach, in which a solvent incorporating a small amount of DIO processing additive is briefly dripped during casting of the perovskite precursor. This films cast on the ITO/PEDOT:PSS substrate by the PAD method exhibited a superior smooth, uniform morphology with high crystallinity and large grain size, which is suitable for large-area devices. And also we fabricated that PHJ PrSCs with perovskite materials by the PAD method may exhibit superior performance with little variation and be applicable to larger area devices.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-469**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Efficient Hole Transporting Materials with Triazole Core for High Efficiency Perovskite Solar Cells

고경국 이재관[1,*]

조선대학교 탄소소재학과 [1]조선대학교 화학교육과/탄소소재학과

Over the past few years, organometal halide perovskite materials have received considerable attention in the scientific community because of the breakthrough of achieving over 18% power conversion efficiency (PCE) for energy conversion devices and their ready availability through efficient solution processing techniques. Alkylammonium lead halides, $(RNH_3)PbX_3$ (R = alkyl, X = Cl, Br, I), are direct band gap materials with hybrid organic-inorganic perovskite structures; they can be synthesized through chemical deposition or spin-casting of precursor solutions. Besides the perovskite materials, hole transporting materials (HTMs) are also one of the most important components because they have considerable influence on the photovoltaic characteristics of perovskite solar cells. In particular, although the spiro-MeOTAD has been widely utilized as HTM for high efficiency perovskite solar cells with PCEs of over 15%, this material still suffer from the expensive synthetic cost because of its multi-step synthesis and difficult purification.As an alternative, we have very recently developed new and cost-effective small molecule HTMs as alternatives to spiro-MeOTAD for high efficiency perovskite solar cells, and in this work we newly synthesized efficient HTMs comprising of triphenyl donor and various acceptors. These synthetic HTMs with donor-acceptor type molecular structures exhibited effective intramolecular charge transfer for improving the hole transporting properties. These synthetically simple and inexpensive HTMs hold promise for replacing the more expensive spiro-OMeTAD.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-470**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of Thiol-capped Au and Pt Nanoparticles Using Modified One-Phase Method

박지수 황다정 김유혁*

단국대학교 자연과학대학 화학과

In the previous work for the preparation of thiol-capped Ag nanoparticles, we modified the one-phase method to prevent the initial formation of Ag(I) thiolate-layered materal from the mixture of AgNO3 and thiols. In this modified method, AgNO3 is added to the mixtures of NaBH4 and thiols in ethanol. This method was so successful so that a modified one-phase method for thiol capped Au and Pt nanoparticles has been explored. This work reports on the characterization of the products by ultraviolet-visible (UV-vis) spectra, X-ray powder differaction (XRD), and transmission electron microscopy (TEM).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-471**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Externally controlled drug release using a gold nanorod contained composite membrane

조민철 정선도 박명환*

삼육대학교 화학과

Versatile drug delivery devices using nanoporous membranes consisting of gold nanorods and dendrimers have been demonstrated to provide light-triggered on-demand pulsatile release from a reservoir containing highly enriched therapeutics for a real patient's needs. The drug release rate is directly correlated with the temperature increase and irradiated energy of a near-IR laser in both static and fluidic devices. This biocompatible platform for on-demand control was further confirmed by in vitro experiments. Interestingly, the different response to stimuli was obtained from each drug in the absence and presence of NIR light, indicating the versatile potential of our on-demand drug delivery system in less-invasive therapies requiring multi-drug delivery strategies. The enhanced delivery system will improve therapeutic efficacy and reduce side effects through regulation of plasma drug profiles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-472**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

N-doped zeolite-templated carbon as a metal-free electrocatalyst for oxygen reduction

권용현 김경수[1,*] 유 룡[2,*]

KAIST 화학과 [1]기초과학연구원 나노물질및 화학반응 연구단 [2]기초과학연구원 나노물질및화학반응연구단

Porous carbons supporting Pt metal are widely used as an oxygen reduction reaction (ORR) catalyst in the cathode of fuel cells and metal-air batteries. But, high cost of the metal is an obstacle in the fuel-cell technology. It is highly desirable to replace the expensive metal by a low-cost metal or other elements. In response to the need, an emerging approach is to use N-doped carbons as an ORR catalyst instead of metal-supporting carbons. This approach is based on the concept that N atoms incorporated into a carbon induce uneven charge density distribution and thereby create catalytic active sites for the ORR.In the present work, we prepared N-doped carbon by hard templating synthesis method using a mixture of acetonitrile and water vapors as N-containing carbon source, and beta zeolite as template. The resultant carbon, denoted by N-doped zeolite-templated carbon (N-ZTC), had a three-dimensionally interconnected, ordered microporous structure with uniform micropore and large surface area. ^{13}C NMR spectroscopy of the carbon showed no other carbon peaks except for sp^2-carbon, indicating that the carbon was likely to have a graphene-like framework. N atoms were incorporated in the carbon at approximately 4.1 wt%. We tested the carbon as an electrocatalyst for the ORR. In the ORR, the N-ZTC showed a notably high current density and a positive onset potential as compared to N-doped reduced graphene oxide. Characterization by Kelvin probe force microscopy indicated that the surface of this carbon also had a lower work function than that of planar graphene nanosheets. The high ORR catalytic performance with the low work function of this carbon seems to come from the high-surface area microporous topology consisting of curved graphene-like walls.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-473**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Topochemical Catalysis of Exfoliated Layered Cobalt(II) Hydroxide for the Synthesis of Ultrapure Co_3O_4 as a Fuel Cell Catalyst

권성윤 이종현*

가톨릭대학교 화학과

Keywords: layered cobalt hydroxide, Fuel cell, Co_3O_4 nanocubeTwo-dimensional nanosheets can be produced by the liquid exfoliation of layered materials, exhibiting improved surface area and unexpected physicochemical properties compared to their bulk materials. Recently, the nanosheets of exfoliated layered metal hydroxides have led to new developments in durable catalysis, multifunctional hybrids, and highly efficient electrocatalysis. We found a novel functionality of exfoliated layers of layered cobalt hydroxide (Ex-NS-$Co(OH)_2$), fresh hydroxide surface and much lower oxidation potential compared to the bulk α-$Co(OH)_2$ particles after the exfoliation. In this study, these novel nanoscopic natures of Ex-NS-$Co(OH)_2$ were used for the surface-assisted synthesis of spinel Co_3O_4 nanocrystal under a simple refluxing condition using aqueous solution of $CoCl_2$ and hexamethylenetetramine (HMT). Importantly, Co_3O_4 nanoparticles are considered as potential alternative of Pt-based materials for efficient oxygen reduction reaction (ORR) catalysts owing to their structural diversity and electrochemical stability. The ORR is crucial in fuel cells and metal-air batteries. Thus, the ORR activity and durability of the current Co_3O_4 nanocrystal were investigated compared to that of commercial Pt catalyst.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-474**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Three dimensional tubular graphitic carbon ('graphene') networks from electrospun polymer fiber mats

구민 이선화[1] **Rodney Scott Ruoff[2,*]**

UNIST 화학과, IBS CMCM [1]기초과학연구원 다차원탄소재료연구단 [2]UNIST 화학과

Three-dimensional (3-D) interconnected graphene networks are, or could be, an interesting material for a variety of potential uses and also for fundamental study. Here, we report about 3-D tubular 'graphene' (thin graphitic carbon) networks. Electrospun polymer fiber mats were made and used as an interconnected porous template to template these graphitic carbon networks. Metal was deposited onto the fibers in the electrospun mats and catalyzed the conversion to the 3-D graphitic carbon. *This work was supported by the IBS-R019-D1.*

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-475**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

UiO-66-type Metal-Organic Framework with Free Carboxylic Acid: Versatile Adsorbents via H-bond for Both Aqueous and Non-aqueous Phases

송지윤 정성화*

경북대학교 화학과

The metal–organic framework (MOF) UiO-66 was synthesized in one step from zirconium chloride and isophthalic acid (IPA) together with the usual link material, terephthalic acid (TPA). UiO-66 with free –COOH can be obtained in a facile way by replacing up to 30% of the TPA with IPA. However, the chemical and thermal stability of the synthesized MOFs decreased with increasing IPA content used in the syntheses, suggesting an increase in the population of imperfect bonds in the MOFs because of the asymmetrical structure of IPA. The obtained MOFs with free –COOH were applied in liquid-phase adsorptions from both water and model fuel to not only estimate the potential applications but also confirm the presence of –COOH in the MOFs. The adsorbed amounts of several organics (triclosan and oxybenzone from water; indole and pyrrole from fuel) increased monotonously with increasing IPA content applied in MOF synthesis (or –COOH in the MOFs). The favorable contribution of free –COOH to adsorption can be explained by H-bonding, and the direction of H-bonds was confirmed by adsorption of oxybenzone in a wide pH range. The versatile applications of the MOFs with –COOH in adsorptions from both polar and nonpolar phases are remarkable considering that hydrophobic and hydrophilic adsorbents are generally required for water and fuel purification, respectively. Finally, the presence of free –COOH in the MOFs was confirmed by liquid-phase adsorptions together with general Fourier transform infrared analyses and decreased chemical and thermal stability. In summary, it was confirmed that UiO-66 with free –COOH can be synthesized facilely in one step from inexpensive IPA and TPA, and the obtained MOFs can be used in various adsorptions, especially in the liquid phase.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-476**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Adsorptiive denitrogenation of a model fuel using metal-organic framework containing free carboxylic acid groups

서필원 정성화*

경북대학교 화학과

Adsorptive denitrogenation was carried with a metal-organic framework from a model fuel having nitrogen containing compounds (NCCs), indole (IND) and quinoline (QUI). For this, UiO-66s, prototypes of MOFs, were applied as adsorbents with or without functionalization of free carboxylic groups. The adsorption capacity of neutral IND was Remarkable improved over the carboxylic group functionalized UiO-66 even though the porosity of the functionalized UiO-66 (UiO-66-COOH) was lower than that of the pristine UiO-66 (103% and 28% based on surface area and weight, respectively). The enhanced performances of UiO-66-COOH could be explained by the formation of H-bond interactions between O (of –COOH) and H (of IND), which was supported by the differences in the adsorption of pyrrole vs. methylpyrrole. Curiously, the adsorbed amount (based on weight) of basic QUI decreased after the introduction of free –COOH on UiO-66, even though favorable acid-base interactions were expected. However, the amount of adsorbed QUI increased by 41% based on surface area. The adsorptive performances of UiO-66s for pyridine were very similar to those for QUI. Therefore, UiO-66-COOH might be also beneficial for the adsorption of basic NCCs, probably because of the existence of acid-base interactions (between N of NCCs and H of –COOH). It is also found that, the effect of free COOH on the adsorption of basic NCCs is generally lower than that of neutral NCCs having hydrogen atoms capable of acting as hydrogen bond donors. From this study, MOFs having free –COOH can be used as potential adsorbents to remove neutral NCCs. Because of their lack of functionality it is particularly important for these adsorbates which are not easy to remove.

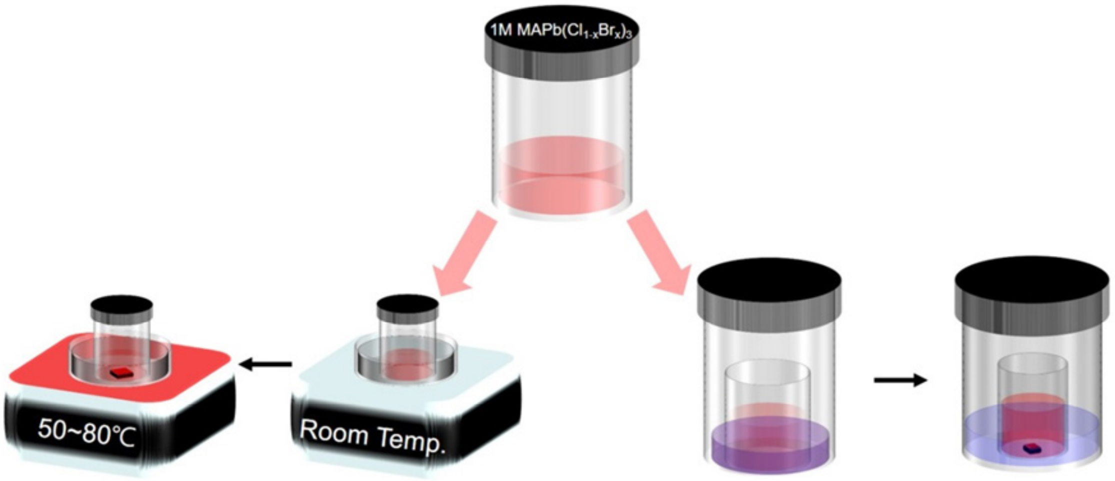
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-477**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fast crystallization of bandgap modulated organic lead halide perovskite single crystals

박대영 정문석*

성균관대학교 에너지과학과

Organic lead halide perovskite has been focused by many scientists due to its excellent properties in photovoltaic and optoelectronics. Especially, perovskite solar cell recorded 20.1% power conversion efficiency despite of short research period. However, high quality of film in devices is crucial for fabricating high performance device. For improving film quality, some researchers fabricated devices based on organic lead halide perovskite single crystal and demonstrated high performance. But, they synthesized only three representative organic lead halide perovskite single crystals(CH3NH3PbX3,CH3NH3 MA, X=Cl, Br, I). For the expansion of applicability, bandgap tuning is essential. Therefore, we prepared bandgap modulated organic lead halide perovskite single crystals (MAPbCl3-xBrx, MAPbBr3-xIx) by changing halogen ratio within 24h using retro-grade solubility property and anti solvent diffusion. Synthesized samples were characterized with XRD, UV-Vis, FT-IR, photoluminescence, TGA, SEM and etc.



$MAPbCl_{3.0}$, Cl/Br 5:1 → 50℃ for **6h**

Cl/Br 2:1 ~ $MAPbBr_{3.0}$ → 80℃ for **6h**

With Anti solvent for **24h**

Anti solvent : Methylene chloride(CH_2Cl_2)

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-478**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Photocatalytic Properties of Oxygen Deficient $SrTiO_3$ Nanoparticles

김경태 강혜지 김유진 허남회*

서강대학교 화학과

$SrTiO_3$ adopts the perovskite-type structure, which has a wide band gap (3.2 eV) and is photocatalytically active only under the UV light irradiation. We have made oxygen vacancies in the $SrTiO_3$ matrix to narrow the band gap of $SrTiO_3$, which results in the absorption of the visible light. The oxygen-deficient $SrTiO_{3-x}$ nanoparticles (NPs) were successfully prepared by the magnesiothermic reduction, in which SrTiO3 NPs and Mg powders are reacted in an evacuated quartz tube. The black $SrTiO_{3-x}$ product was characterized by transmission electron microscopy, elemental mapping, X-ray diffraction, thermo gravimetric analysis, UV-visible spectroscopy and X-ray photoelectron spectroscopy. The photocatalytic results suggest that oxygen vacancies on $SrTiO_3$ play a major role in the visible light absorption and enhanced photocatalytic activity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-479**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effective parameters on liquid-phase adsorption of aromatics over a metal–organic framework and activated carbon: hydrophobicity/hydrophilicity of adsorbents and solvent polarity

Biswa Nath Bhadra 정성화*

경북대학교 화학과

Solvent polarity and hydrophilicity/hydrophobicity of adsorbents were considered parameters on which the liquid phase adsorption of aromatics might be affected. Thiophene, pyrrole, and nitrobenzene were selected aromatics because of their very low acidity or basicity. On the other hand, two highly porous adsorbents, a metal-organic framework (MOF, MIL-101) and activated carbon (AC) were used. Selected adsorbates were tested to estimate possible applications of the adsorbents in liquid-phase adsorptions to estimate possible applications of the adsorbents in adsorptive desulfurization (ADS), adsorptive denitrogenation (ADN), and water purification, respectively. MIL-101 adsorbed all the three adsorbates more effectively with decreasing solvent polarity, and AC with increasing solvent polarity. This behavior can be explained by the hydrophilicity of MIL-101 and hydrophobicity of AC, which was confirmed by measuring the hydrophobicity indexes. The preferential adsorptions of the adsorbates over MOF and AC might be explained by polar-interactions and hydrophobic-interactions respectively. Moreover, it can be concluded that adsorptions in non-aqueous phases including ADS and AND, hydrophilic MOFs are preferential ones. Finally, adsorptions of aromatics from water, it is necessary to increase the hydrophobicity of a MOF to elucidate applicability of MOFs in water purification.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-480**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Adsorptive denitrogenation of model fuel by sulfonated metal-organic framework: dual effect of hydrogen-bonding and acid−base interaction

imteaz ahmed 정성화*

경북대학교 화학과

A sulfonated metal-organic framework (MOF), UiO-66-SO3H was used for the adsorptive removal of nitrogen containing compounds (NCCs) indole (IND) and quinoline (QUI) for the first time. The adsorption of IND was increased with increasing content of -SO3H in UiO-66. The favorable effect of the -SO3H group on the adsorptive removal of IND could be explained by hydrogen bonding between the O of -SO3H and the H of IND, which was firmly supported by the adsorption of pyrrole and methylpyrrole and by theoretical calculations. The application of an -SO3H group in the adsorptive removal of neutral IND is meaningful since neutral nitrogen-containing compounds are not easy to remove and since UiO-66-SO3H is reusable after simple washing with ethanol. At low concentration (

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-481**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of $YFe_{1-x}Mn_xO_3$ ($0.1 \leq x \leq 0.4$) and their photocatalytic activity

부충헌 김다혜 정동운*

원광대학교 화학과

전이금속 산화물인 $YFeO_3$ 에서 Fe 를 미량의 Mn 으로 치환시킨 $YFe_{1-x}Mn_xO_3$ ($0.1 \leq x \leq 0.4$)를 용액합성법으로 제조하였다. 제조한 시료들은 XRD, XPS, UV-visible 장비를 이용해 구조 및 성질을 분석하였다. Mn 의 치환량이 증가 할수록 가시광선 영역에서의 흡광도가 증가하였는데, 이는 Mn 의 치환량이 증가할수록 띠 간격이 감소하여 나타나는 결과로 여겨진다. 가시광선 영역에서 흡광을 통한 유기물 분해를 비교하기 위해 각 시료들의 광촉매 활성 실험을 진행 하였으며, Mn 의 치환량이 증가 할수록 광촉매 활성 또한 증가한다는 것을 관찰 하였다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-482**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enhancement of photocatalytic activity over black-BiOCl/Bi_2O_3 heterojunction

김다혜 부충헌 정동운[*]

원광대학교 화학과

Bi_2O_3 로부터 용액합성법을 통해 BiOCl/Bi_2O_3 헤테로접합 화합물을 다양하게 제조하였다. 얻어진 BiOCl 화합물은 열 또는 빛 에너지에 의해 black-BiOCl 로 변화하였으며 BiOCl 화합물의 열처리 시간이 증가 할수록 가시광선 영역에서의 흡광도가 증가하였다. 이는 BiOCl 화합물에 가해지는 열 또는 빛 에너지의 양이 증가할수록 산소의 이탈이 발생하여 띠 간격이 감소하는 결과로 여겨진다. black-BiOCl/Bi_2O_3 헤테로접합 화합물들은 기존의 BiOCl/Bi_2O_3 헤테로접합 화합물에 비하여 더욱 향상된 광촉매 효과를 나타냈다.

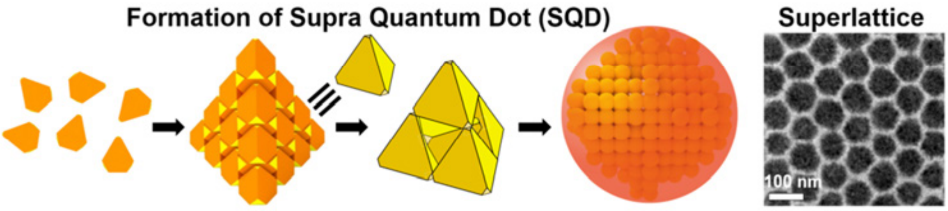
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-483**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Formation and Stepwise Self-assembly of Cadmium Chalcogenide Nanocrystals to Colloidal Supra-Quantum Dots

정상화 김성지*

POSTECH 화학과

Nearly monodisperse colloidal superstructures of cadmium chalcogenide quantum dots (QDs) were reported as the three-dimensionally(3D) assembled QDs by pyrolysis-based synthesis. The superstructures, which we named as 'supra quantum dot (SQD)', are typically composed of hundreds of a-few-nm-sized QDs assembled by oriented attachments. The synthesis route is quite universal and can be extended to CdS, CdSe, CdTe, and CdSeTe alloy. The size of SQD can be tuned from tens of nm to over a hundred nm. In the case of CdSe SQD, zinc-blende seeds (primary QDs) act as the building block for the formation of the 3D assembled SQDs with discrete intermediates nanostructures. Primary seeds, 4 nm tetrahedral shaped QDs, assembled into a large tetrahedron of 20 nm. The 20 nm tetrahedrons, in turn, self-assembled into a larger tetra-hedron of 40 nm. The discrete-in-size and sequential assemblies were followed by conventional growth from the remaining precursors and ripening within the particles to result in spheroidal SQDs. SQDs allow surface ligand exchanges without losing the integrity. Size-selective precipitations of SQDs can provide monodisperse SQDs that can assemble into ordered superlattices. The size and composition tunability SQDs and their capability to form superlattices can provide a new solution-processible building block for 'metamaterials' with programmable physical and chemical properties.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-484**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Laser Induced ZnO Nanorods / Reduced Graphene Oxide Composites for Supercapacitor

정재민 이민형*

경희대학교 응용화학과

Development of advanced materials and structures for supercapacitor is critical to achieve new energy storage devices with high power density. Metal oxide/graphene hybrids can increase chemical and electrical coupling effects, and high surface area and electrical conductance of graphene are also attractive points as an advanced material for electrochemical devices. In this work, we present the growth of ZnO nanorods/reduced graphene oxide composites on PET film via laser assisted bottom-up synthesis (LABS) which was followed by hydrothermal process below 100 ℃. The complexes could be used as supercapacitor electrodes due to its pseudo capacitance (ZnO) and electric double layer capacitance (graphene). And these high electron mobility and surface of volume ratio of both materials brought improving of capacitor performance.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-485**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Gold Nanoparticles on Layered Double Hydroxide Nanosheets and Its Electrocatalysis forGlucose Oxidation

권영민 박소연 이종현*

가톨릭대학교 화학과

Gold nanoparticles have exhibited good anti-poisoning property and more negative oxidationpotential during the electrocatalysis of glucose oxidation. However, the fast aggregation ofgold nanoparticles during the synthetic and catalytic process has increased the requirementsfor well-defined nanoscopic supporting materials. Recently, two-dimensional nanosheet ofexfoliated layered double hydroxide (LDH) of 1–2 nanometer thick layers has emerged as anew type of solid support to immobilize the diverse metal nanoparticles, because of the largemetal hydroxide area, good bio/chemical stability, and highly charged positive potential. Wedeveloped a facile method to deposit spherical Au NPs with the diameter range of 2–10 nmon the entire surface of LDH nanosheets by the in situ chemical reduction of $HAuCl_4$ with$NaBH_4$. This strong reducing chemical quickly forms Au NPs on the LDH nanosheets;however, the Au NPs were tightly immobilized on the LDH nanosheet, because of the highlycharged positive potential of LDH surface. Here, we employed the Au/LDH nanosheet as theactive material for the electrochemical oxidation of glucose. The Au/LDH-modified electrodeexhibited significant and intense anodic peaks for glucose oxidation both in the anodic andcathodic scans, at 0.26 and 0.13 V, respectively. The results strongly demonstrate that thenanoscopic nature and dense positive charges of LDH nanosheet stabilized the Au NPs tomaintain their inherent properties during the synthesis and electocatalysis.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-486**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Scandium-triflate/metal-organic frameworks: remarkable adsorbents for liquid phase desulfurization and denitrogenation

Nazmul Abedin Khan 정성화*

경북대학교 화학과

There is a considerable demand to reduce the content of sulphur- and nitrogen-containing compounds in fuels like diesel and gasoline to a low level to prevent air pollution and deactivation of catalysts. Metal-organic frameworks (MOFs), with the incorporation of scandium-triflate (Sc(OTf)3) have been investigated to adsorb benzothiophene (BT), dibenzothiophene (DBT), quinoline (QUI) and indole (IND) from liquid fuel. A remarkable improvement in the adsorption capacity (about 65% based on the weight of adsorbents; 90% based on the surface area of the adsorbents) was observed with the Sc(OTf)3/MOFs compared to the virgin MOFs for the adsorption of BT from liquid fuel. The basic QUI was also adsorbed preferentially onto the acidic Sc(OTf)3/MOFs. However, non-supported Sc(OTf)3 showed negligible adsorption capacities. The improved adsorptive performance for BT, DBT and QUI might be derived from acid–base interactions between the acidic Sc(OTf)3 and basic adsorbates. On the other hand, the Sc(OTf)3, loaded on MOFs, reduced the adsorption capacity for neutral IND due to lack of interaction between the neutral adsorbate and acidic adsorbent and the reduced porosities of the modified adsorbents. The reusability of the adsorbents was found satisfactory up to the fourth run. Based on the result, it is suggested that metal-triflates, such as Sc(OTf)3 can be effective sites for the adsorption of various basic organosulfur and organonitrogen compounds.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-487**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fabrication of Superhydrophobic Filter Paper with Hydrophobic Iron Fatty Acids/PS Composite Solution

이우희 안용현[1,*]

단국대학교 자연과학대학 화학과 [1]단국대학교 화학과

Paper is composed of fibrous cellulose, which makes it a cheap and biodegradable material. Due to its physical property of hydrophilicity, papers are widely employed when high wettability is required. Surface modifications can be applied to induce superhydrophobic properties, which by definition generate a water contact angle (WCA) of >150o and a water slide angle (WSL) of < 10o. The lotus leaf is a naturally occurring example of superhydrophobic surfaces, featuring self-cleaning capabilities. In this experiment, hydrophobic iron fatty acid particles/PS composite coating solutions were prepared and used to fabricate a superhydrophobic coating on filter paper. After surface modification using a spray coating method, the superhydrophobic paper could be applied for oil/water separation. Furthermore, various hydrophobic iron fatty acids can be synthesized and used for the preparation of composite coating solutions. By simply spraying a composite coating solution (iron fatty acid/PS in THF) on the cellulose fiber surface, a superhydrophobic filter paper is fabricated. The iron fatty acid derivative particles are synthesized via a chemical reaction between iron (III) chloride hexahydrate and fatty acids. The superhydrophobic filter paper was shown to provide a WCA of 155°.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-488**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Adsorptive removal of phenol from fuel over hydroxyl-functionalized Cr based MIL-101 via H-bonding

SARKER MITHUN Biswa Nath Bhadra 정성화*

경북대학교 화학과

In order to understand the possible application of MOFs in fuel purification, adsorption of phenol from n-octane (a model fuel) over hydroxyl group functionalized Cr based metal-organic framework, HO-MIL-101(Cr), was investigated and compared with virgin MIL-101(Cr) and commercial activated carbon. A remarkable enhancement in phenol adsorption capacity (~2.7 and ~3.7 times) was observed over the functionalized-MIL-101(Cr) and AC respectively. Despite the porosity of the MOF was decreased noticeably by grafting ethanolamine (EA) on coordinatively unsaturated sites on MIL-101, the adsorption capacity increased noticeably. The H-bonding was applied to explain the increased adsorption capacity of phenol on EA-grafted MIL-101 (HO-MIL-101). To understand the possible direction of H-bonding, adsorption of a phenol derivative (anisole) was also conducted. The obtained results for adsorption of phenol and anisole on MIL-101 and HO-MIL-101 were compared which suggest that H-bonding occurs between the H-atom of the phenolic –OH and the O-atom of HO-MIL-101. The used HO-MIL-101(Cr) can be easily regenerated by simple washing with diethylether and reused for adsorptive removal of phenol from fuel. Therefore, suitable pre-/post-fictionalization of the virgin MOFs would broaden the application of MOFs in removing phenol or other organic impurities from fuel.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-489**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Surface Modification Route For Biocompatible Magnetic Iron−Nickel Nanocrystals

권준영 이재범[1,*]

부산대학교 인지메카트로닉스공학과 [1]부산대학교 광메카트로닉스공학과

Bimetallic magnetic iron-nickel (FeNi) nanocrystals (NCs) were synthesized through a one-pot synthetic wet chemistry method, and the morphology of the resulting NCs can be adjusted by changing the molar ratio of chemical attendees during the experimental processes. The obtained FeNi NCs can be redispersed in water medium though the phase works by using the ligand exchange procedures of cysteine (Cys), 5-aminovaleric acid (5AA), and glutathione (GSH), respectively. The synthesized NCs exhibited excellent magnetic properties with Hc (magnetic fields, ≈10−3 T) and μa (initial permeability of up to 105). Furthermore, linear sweep voltammetry (LSV) polarization curves revealed a low overpotential of −0.47, −0.44, and 0.15 V and a current of 105.7, 97.8, and 209 mA for the Cys-, 5AA-, and GSH-FeNi NCs, respectively. This indicated a relatively high catalytic activity of these NCs in the hydrogen evolution reaction (HER). The different cell lines (AGS, HepG2, MG63, NCI-H460, and SK-MEL-2) exposed to FeNi NCs for 5 days exhibited >87% viability at concentrations of up to 50 μg mL−1, which was indicative of excellent biocompatibility. The resulting FeNi NCs offer a facile synthetic route to fabricate monodispersed NCs. The biocompatibility of these NCs should also enable their application in electrocatalysis and biological applications.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-490**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of FeOF/Reduced Graphene Oxide Nanocomposite as a Cathode Material for Lithium-Ion Batteries

박미지 김종식*

동아대학교 화학과

Among various energy storage devices, lithium ion batteries (LIBs) have been used as the promising power source for a wide range of applications including hybrid electric vehicles (HEVs) and electric vehicles (EVs). Although LIBs have some advantages of its high energy density, high voltage, and long lifespan, it is still required to improve the electrochemical performance such as high specific capacity of the cathode material. Iron oxyfluoride (FeOF) is one of the attractive candidates as a cathode material because of a higher theoretical capacity of 885 $mAhg^{-1}$ than FeF_2 (571 $mAhg^{-1}$) and FeF_3 (712 $mAhg^{-1}$). However, FeOF exhibits poor rate capability and cycling stability due to its low diffusion coefficient of lithium-ions and poor electrical conductivity. Reduced graphene oxide (r-GO) has been used to enhance the electrical conductivity and to avoid agglomeration of cathode materials. In this study, FeOF nanoparticles are decorated on the r-GO. The amount of the r-GO is adjusted to obtain the optimal electrochemical performances. The synthesized FeOF/r-GO nanocomposites are thoroughly characterized by XRD, FT-IR and SEM analyses. The nanocomposites show the improved discharge capacity and cycling stability compared to bare FeOF.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-491**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Generation of complex nanostructures with high aspect-ratio, high resolution and high area-density from conventional single block copolymer nanostructure

전환진

KAIST 나노종합기술원

Creation of high resolution nano-patterns with high-aspect-ratio, high areal density and tunable features is one of the most important issues in block copolymer (BCP) research. This is particularly difficult in BCP assembly, because of its thermodynamically limited BCP morphologies and nature of ultrafine pattern dimension for conventional pattern transfer methods. In this study, we introduced the new concept BCP lithography method by combining the secondary sputtering phenomenon during ion-bombardment process, which can enable the many different shaped nanopatterns with enhanced feature dimension, high-aspect-ratio (~10) and high areal density (doubling) of nano-patterns from single BCP structure. Complex patterns including doubled walls, nanotube, nanocrescent, cup-shape, U-shaped and L-shaped line arrays with 10-nm-scale resolution, aspect-ratio of ~10 and doubled areal density were facilely fabricated from conventional single BCP nanostructure with 10-nm-scale resolution, aspect-ratio of ~1 without further complicated process.

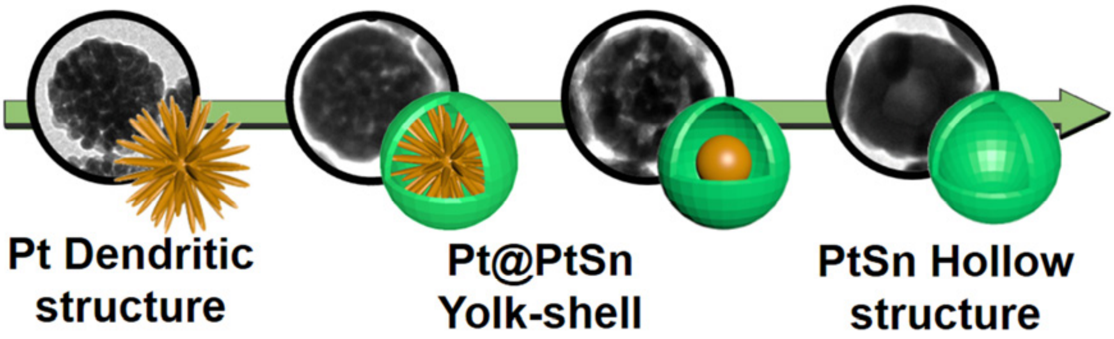
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-492**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Formation of hollow Pt-based alloy nanoparticles from hetero atom deposition on Pt dendritic structures

권태현 박종식 이광렬*

고려대학교 화학과

Hollow nanoparticles with a high surface-to-volume ratio have found various applications in catalysis, sensors, and energy storage, and thus new synthetic routes to obtain these structures are of great interest. One of the best-known synthetic route to hollow nanostructure is the utilization of the Kirkendall effect, which, however is not useful for systems with a slow diffusing-out core such as Pt and fast diffusing-in surface elements such as Sn. Herein, we report a counterintuitive formation of hollow PtSn nanostructures by reacting dendritic Pt nanostructures with Sn precursors.



대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-493**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enhancing electrocatalytic property toward oxygen reduction reaction in PtNi alloys by acid etching

권혁부 박종식 이광렬*

고려대학교 화학과

There have been great interests on Pt based catalysts because of their outstanding performance in electrocatalytic reactions. However, the high cost of platinum has limited its practical use as electrocatalyst. In order to overcome this limitation, alloying with other transition metals has been extensively studied because the high production cost can be curbed and higher catalytic activity can be gleaned. Among the various Pt-M alloy compositions, Pt_3Ni composition has been particularly promising as ORR catalysts. Herein, we report a convenient route to expose highly active bare Pt_3Ni surface of surfactant protected PtNi@Ni nanorods.

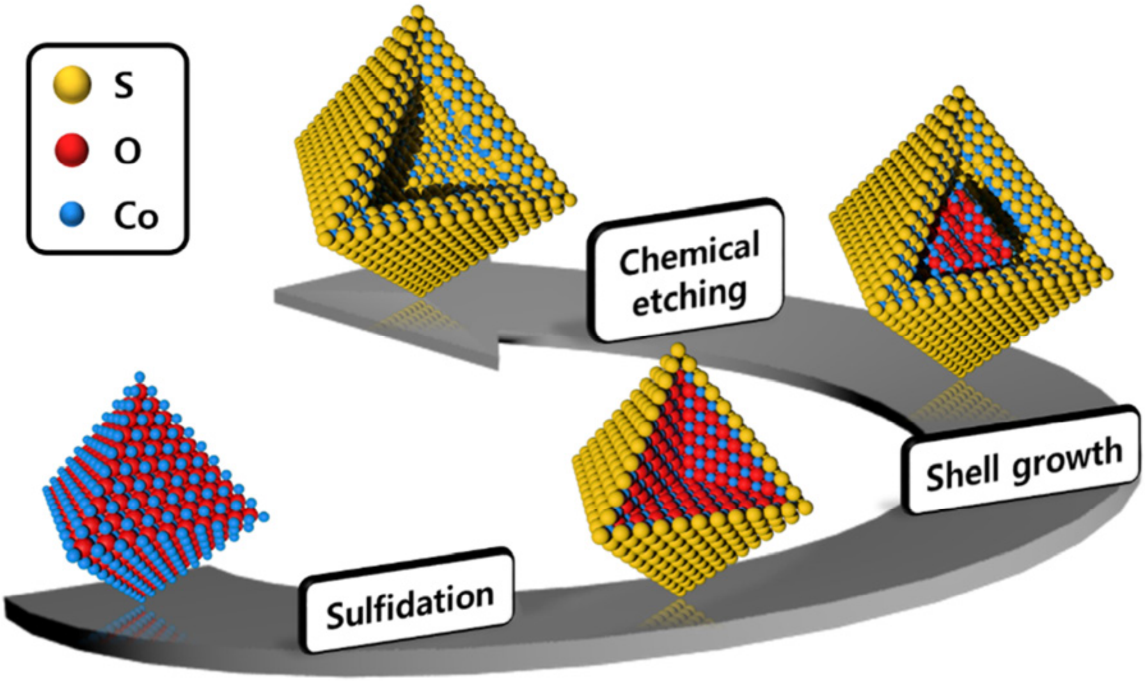
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-494**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Co_9S_8 octahedral nanocage

김준 이광렬[*]

고려대학교 화학과

Cobalt sulfide (Co_9S_8) with unique hollow octahedral morphology was synthesized via template-mediated sulfidation of CoO followed by removal of the CoO core by chemical etching. The formation of Co_9S_8 shell on CoO is facilitated by Kirkendall effect, and the thickness of the shell can be controlled by adjusting the sulfidation temperature. The as-synthesized CoO@Co_9S_8 is treated with acid to remove the core and yield Co_9S_8 octahedral nanocages.



일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-495**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of metal chalcogenides from single precursors

김태경 이광렬*

고려대학교 화학과

Nanostructured metal chalcogenides(NMCs) have received a great attention in a variety of applications, which includes fuel cells, solar cells, supercapacitors, theromoelectric devices and sensors. In this study, we developed a facile synthetic method of NMCs from appropriate precursors, namely, metal thio- & seleno-cyanate precursors. Phase selective NMCs could be obtained from single metal thio- & seleno-cyanate precursors in large scales.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-496**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Nanoframe of double layered structural features with excellent electrocatalytic activity toward oxygen evolution reaction

박종식 이광렬*

고려대학교 화학과

Noble metal nanoframes have attracted a great interest from numerous research groups due to their high catalytic surface area, stemming from three-dimensional molecular accessibility. Previously, hollow, frame nanostructures have been prepared by multi-step template-mediated growth, which involves the formation of template, growth on the template and finally removal of the template. Herein, we describe a convenient one step synthetic method of development of a unique double-layered nanoframe structure with high activity and stability toward oxygen evolution reaction.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-497**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile Synthetic Route to Reduced Graphene Oxides and Their Energy Storage Properties

장혜련 백승민*

경북대학교 화학과

Reduced graphene oxide has already gathered considerable interest in the fields of science, engineering and biotechnology because of interesting textural properties. Synthesis of reduced graphene oxide via microwave irradiation was relatively quick and simple as compared with all the other reduction methods, and was applied in this study. The XRD result of microwave-reduced graphene oxide(or MrGO) represented the disappearance of graphene oxide peak, and showed typical amorphous XRD pattern for reduced graphene oxide. The Raman spectroscopy showed intensity ratio of MrGO, which was close to that of GO because of oxygen functional group. The TEM image showed thin nanosheets that consisted of single and/or multi-stacked layer, and confirmed sporadically crumpled and folded configuration. The electrochemical measurements to investigate energy storage properties of products clearly showed that the disordered structure stored much higher amount of Na ions and had the enhanced rate capability in higher current density. MrGO, possessed exceptional electrochemical property, could be a key role in energy storage system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-498**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A New Hollow Nanostructure between Titanate and Graphene Oxide for Enhanced Photocatalytic Performance

이원재 백승민*

경북대학교 화학과

The titanium dioxides have highly attracted both scientific and industrial interests due to their promising application in photocatalysis. Also, the graphitic carbon can be an effective co-catalyst due to its feature as an electron scavenger. In this study, the hollow structured titanate/graphene oxide was synthesized via self-restacking by using electrostatic interaction onto polystyrene bead as soft template. In the electron microscopy images, the obtained samples show that the nanosheets were covered on the polymer beads, and then, the products were sintered to form hollow sphere. According to energy dispersive spectroscopy, the carbon and titanium was homogeneously distributed in hollow spheres. The photocatalytic degradation performances of organic pollutants show that the present product could be used as a potential photocatalyst with enhanced performance.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-499**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Compositionally well-defined multimetallic icosahedral nanocrystals: Ru-based dual core-shell nanoframes as high-performance electrocatalysts for Oxygen Evolution Reaction

오아람 이광렬*

고려대학교 화학과

Ruthenium-based nanostructures have drawn great attention due to their excellent catalytic activity in oxygen evolution reaction. However, it is still a challenge to improve their stability during electrochemical reaction. In order to solve the problem, here we developed a rational design of Ru-based multimetallic nanocrystals by understanding the nanostructure growth kinetics. The Ru-based alloy nanoframes show the excellent catalytic activity and durability for oxygen evolution reaction in alkaline and acidic media.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-500**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Layered Trirutile/Nickel Oxide Hybrids for Photocatalytic Application

우준혁 백승민*

경북대학교 화학과

It is known that the layered trirutile compounds have outstanding photocatalytic properties. Also, they have been consistently researched because of improved physical and chemical properties obtained by hybridization with other materials. In this study, the layered trirutile compound, LiTaWO6, was synthesized by a solid-state reaction, and then, exfoliated into nanoscale colloids by intercalating tetra(n-butylammonium) hydroxide. The exfoliated nanosheets were hybridized with nickel oxide nanoparticles. We confirmed the structure of the exfoliated nanosheet using X-ray diffraction and transmission electron microscopy. The UV-vis diffuse spectra were measured for investigating the bandgap energy of products. The photocurrent measurements represent that the present hybrids could be used as a potential photocatalyst.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-501**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of unprecedented nanostructures by using copper sulfide template and their applications

윤동환 이광렬*

고려대학교 화학과

Nanostructures are known to have unique material properties depending on their morphology and therefore the design and synthesis of nanostructures with controlled morphology have received a great attention. We discovered that shape-controlled copper sulfide nanocrystals can serve as unique template platforms for unprecedented nanostructures with interesting material properties. Herein we demonstrate the facile synthesis of various nanomaterials by using copper sulfide nanotemplate and their application in catalysis and nano-optics.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-502**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of iridium oxide 2D hollow nanostructures

이재영 윤동환[1] 이광렬[1,*]

고려대학교 화학과 [1]고려대학교 화학과

The acquisition of renewable energy from hydrogen fuel is feasible by electrolysis of water into oxygen and hydrogen fuels. However, the slow kinetics of oxygen evolution reaction (OER) is the obstacle to water splitting. Iridium oxide (IrO_2) nanoparticles are known as promising OER electrocatalysts which can improve the efficiency of fuel generation technologies. Besides, hollow nanoparticles have drawn great attention due to their high surface-to-volume ratio which enhances the catalytic activity of water electrolysis. Herein we demonstrate a synthetic methodology for iridium oxide (IrO_2) 2D hollow nanostructure and its application toward water splitting.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-503**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

.Fabrication of TiO_2/RuO_2 Hollow Nanostructures with Enhanced Energy Storage Properties

천유경 백승민*

경북대학교 화학과

.Because TiO_2 has the high volumetric and gravimetric energy density, recently it has been studied as an anode material of sodium ion battery. The changed morphology of titanium oxide could lead to an interesting electrochemical property. In this study, nanosized TiO_2 and RuO_2, building blocks to construct a new nanostructure, were fabricated into the hollow structure, which was applied to sodium ion battery. The physicochemical properties of products were characterized by SEM, TEM, XAS, EDS, and XRD analysis. From TEM image, it was confirmed that the thickness of the shell for hollow structure was extremely nanosized. Morphology of the products was confirmed by SEM, showing that the empty circular shape was maintained after the bead mold was removed. Remarkably, XRD and XAS results showed that the TiO_2 phase of a hollow nanostructure was successfully transformed to the rutile structure after the hybridization with RuO_2. According to the electrochemical measurements, the product have more superb energy storage properties, in comparison with those of other starting materials, due to the smaller volume change of TiO_2 and high electrical conductivity of RuO_2.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-504**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile Synthesis of semiconducting and plasmonic Cu_3P platelets

주진환 이광렬*

고려대학교 화학과

Copper phosphide has a great potential for the usage in photocatalytic hydrogen evolution due to small band gap and plasmonic absorption. Because of plasmonic effect, copper phosphide can be activated by not only visible light, but also near IR light (~2000 nm). However, the previous synthetic methods of Cu_3P platelets require expensive and dangerous materials such as PH_3 gas and yellow phosphine. This synthetic limitation is suppressing further research of Cu_3P. Herein, we report an easy synthetic strategy for Cu_3P platelets without dangerous materials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-505**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Lanthanide metal assisted formation of PtNi nanoframe structure from Ni rich rhombic dodecahedral nanoparticle with great electrocatalytic activity towards oxygen reduction reaction

진하늘 이광렬*

고려대학교 화학과

Nano-sized catalysts with frame morphology have been intensively studied in recent years because of their excellent electrocatalytic performance. The regioselective growth and template removal can lead to frame nanostructure in principle. However, it is not so easy to prepare frame nanostructure owing to the lack of our understanding of crystal growth. Herein, we synthesized rhombic dodecahedral PtNi nanoparticles via surface stabilization of Ni nanocrystal by lanthaide ion deposition and growth of Pt on un-coated Ni surface. Specifically, lanthanide metals help regioselective growth of Pt by preventing {111} and {110} facets on rhombic dodecahedral PtNi nanoparticle. PtNi frame nanostructures can be obtained from the etching of Ni in acidic solution and the nanostructures exhibit enhanced catalytic activity on oxygen reduction reaction (ORR).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-506**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

2D Ni-Ni_3S_2 Nanostructures on Ni foam with Unusually Small Tafel Slope towards Oxygen Evolution Reaction

Nitin Chaudhari 이광렬*

고려대학교 화학과

Uniform spider web-like Ni film-Ni_3S_2 and honeycomb-like Ni_3S_2 structures were deposited on nickel foam (Ni_3S_2/NF) by a facile one-step hydrothermal synthetic route. When used as oxygen evolution electrode, the spider web-like Ni-Ni_3S_2/NF due to the large exposed surface area exhibits excellent catalytic activity and stability with an over-potential of ~ 310 mV to achieve at 10 mA/cm^2 and Tafel slope of 63 mV/dec in alkaline media, while honeycomb-like structure, without Ni-film, does not exhibit such material characteristics. This low Tafel value makes Ni-Ni_3S_2/NF one of the best non-precious nickel sulfide-based OER catalysts. The results point to the fact that performance of the metal sulpide electrocatalysts might be fine-tuned and optimized with morphological and composition controls.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-507**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Magnetic iron oxide nanoneedles containing multi-metallic nanoparticles for the removal of toxic organic pollutant

전효경 이하진* 김지선[1]

한국기초과학지원연구원 서울서부센터 [1]이화여자대학교 화학나노과학과

Multi-metallic nanoparticle-contained magnetic iron oxide nanoneedles (mIO-M) were successfully synthesized by a successive coating of dopamine, metal nanoparticles (NP) such as Au, Ag and Pt, and iron oxide nanoneedles on magnetic core. The structure of the mIO-M was characterized using field-emission scanning electron microscopy, transmission electron microscopy. By controlling composition of noble metal ion precursors, mono-metallic, di-metallic and tri-metallic mIOs could be prepared. The mIO-Ms exhibited excellent performance of catalytic activity for the reduction of 4-nitrophenol showing the reduction was completed within 6 min. Furthermore, the magnetically recyclable nanocatalysts were readily separated using an external magnet and reused up to 5 times without loss of the catalytic activity. The catalytic effect on the different composition and content of the metal NPs and the pHs will be further studied.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-508**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of ultrathin Pd decahedron with enhanced electrocatalytic performance

이영욱 한상우*

KAIST 화학과

The various applications of Pd nanocrystals were reported in fuel cell, organic catalysis, SERS and hydrogen storage materials application. Among others, synthesis of Pd nanocrystal is important because this has different properties as per the particle shape. Especially, the thin film nanoparticle has optical property. Also the decahedron was reported to have high electrocatalysis due to twined boundary. We demonstrate that unreported ultrathin Pd decahedral could be exclusively prepared with generally controlled nanoparticles. The ultrathin Pd decahedral exhibited efficient optical, electrocatalysis and surface-enhanced Raman scattering activities due to their unique optical characteristics.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

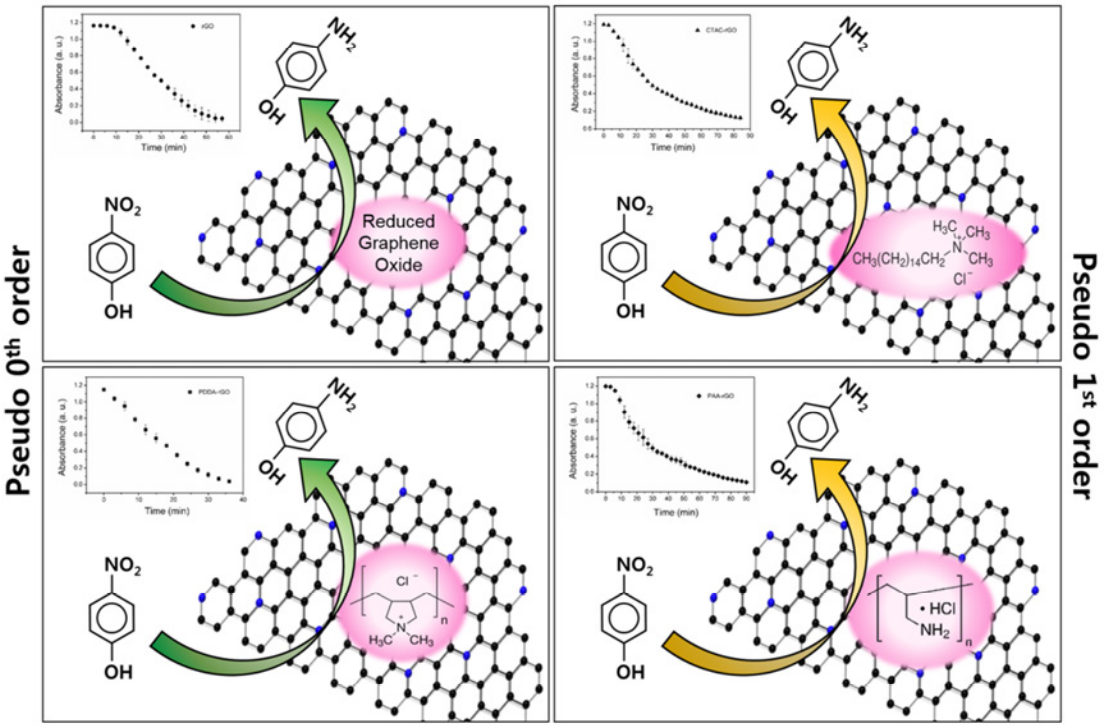
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-509**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Graphene-based Non-metallic Carbocatalysts in Electron-Transfer Reactions

송재은 한상우*

KAIST 화학과

We report an informative strategy to both stabilize and electronically modify reduced graphene oxide (rGO) with electron-accepting capping agents [e.g., poly-(diallyldimethylammonium chloride) (PDDA), cetyltrimethylammonium chloride (CTAC), and poly-(allylamine hydrochloride) (PAA)] in carbocatalysis. The surface-modified rGOs with these positively-charged organic molecules possessing an intramolecular charge-transfer capability were directly applied to metal-free reductions of 4-nitrophenol and ferricyanide. The functionalization of the rGO surface with these capping agents influenced the overall reduction kinetics by controlling the induction time, enhancing the catalytic activity, and changing the reaction order compared to the reduction kinetics of bare rGO and GO. As the reaction kinetics were highly related to the way the capping agents were functionalized on rGO, our simple modification approach can pave the way to rationally designing rGO-based non-metallic catalysts.


Pseudo 0th order
Pseudo 1st order
rGO
CTAC-rGO
PDDA-rGO
PAA-rGO
Absorbance (a. u.)
Time (min)
NO2
OH
NH2
Reduced Graphene Oxide
H3C CH3
CH3(CH2)14CH2 N CH3
Cl⁻
Cl⁻
H3C N CH3
n
• HCl
NH2

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-510**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The influence of the inorganic filler in EMC for the reflectivity of LED

김성덕 정동운*

원광대학교 화학과

EMC(Epoxy molding compound)는 LED(Light emitting diode)의 반사체로 사용되는 화합물이다. EMC 에 첨가하는 무기화합물의 종류에 따라 LED 에서 발생하는 빛의 반사율이 영향을 받는다. 현재 filler 로 사용되는 TiO_2/SiO_2 에 zeolite 및 quartz 입자를 첨가하여 이들의 초기반사율과 시간에 따른 반사율을 측정하였다. Zeolite 와 quartz 입자를 첨가한 경우 초기반사율은 약간 저하되었으나 시간 경과에 따른 반사율 저하가 감소되는 결과를 얻었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-511**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Lithium insertion into $SrTa_2O_6$ and ionic conductivity of $Li_xSrTa_2O_6$ ($x = 0.1-0.5$)

한현동 김영일[*]

영남대학교 화학과

Lithium insertion into β-$SrTa_2O_6$ was carried out by heating with Li_2CO_3 in air at 600℃ for 12 h, where single phase $Li_xSrTa_2O_6$ was obtained up to $x = 0.4$. Powder X-ray diffraction indicated a gradual transition from orthorhombic to tetragonal with the increase of x in $Li_xSrTa_2O_6$. Ionic conductivity of $Li_xSrTa_2O_6$ was measured by ac impedance spectroscopy in N_2 in the temperature range of 30-360 ℃. As revealed by the equivalent circuit analysis, the ionic conductivity increased with the Li content. At 360 ℃, the ionic conductivities were measured to be $10^{-6.7}$ S/cm, $10^{-5.0}$ S/cm, and $10^{-4.7}$ for $x = 0.2$, 0.3, and 0.4, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-512**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and characterization of Ni@Co@Ru nanosandwich

황혜윤 이광렬*

고려대학교 화학과

Shape control of nanoparticles is considered as important challenge because nanoparticles show different performance depending on their facets. Herein, we have demonstrated that two shapes of RuNiCo nanoparticles can be formed by kinetic control. One is sandwich shape (Ni@Co@Ru nanosandwich) obtained from fast reduction of precursors while the other is sphere shape synthesized from slow reduction of precursors. Ni@Co@Ru nanosandwich with core-shell structure is composed of Ni core, Co inner shell and Ru outer shell. The resulting unique structure of Ni@Co@Ru nanosandwich showed improved electrocatalytic activity toward oxygen evolution reaction (OER).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-513**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Acridine Modified Benzofuropyridine and Benzothienopyridine Derivatives and Their TADF Properties

김효정 이석중*

고려대학교 화학과

Thermally activated delayed fluorescence (TADF) has been gradually considered as an alternate for fluorescence and/or phosphorescence based OLEDs. It uses not only singlet but triplet excitons with an efficient internal conversion from the triplet excited state (T_1) to the singlet excited state (S_1) through reverse intersystem crossing (RISC). Therefore, TADF materials have small energy gaps between singlet and triplet excited states (ΔE_{ST}). With a structural modification between donor and acceptor, the restricted HOMO-LUMO overlap can be achieved. In here, we report on the synthesis and the photoluminescence characteristics of acridine modified benzofuropyridine and benzothienopyridine derivatives, employing TADF mechanism with aforementioned structural modification between acceptors (benzofuropyridine and benzothienopyridine) and donors (dimethylacridine) to promote a small ΔE_{ST} between S_1 and (T_1) states. Furthermore, the heterocyclic acceptors are decorated by two dimethylacridine groups known to display high T_1 state which is expected to support further for the small ΔE_{ST}. Due to their distorted molecular structure, both compounds 1 and 2 exhibit well-separated HOMO-LUMO energy levels, small ΔE_{ST} and long lifetime of fluorescence that result in excellent TADF performance.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-514**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Rhodium based ternary sulfide hollow structure for electrochemical hydrogen evolution reaction

양유진 윤동환 이광렬*

고려대학교 화학과

The production of H_2 with electrocatalytic water splitting is one of the key solutions of renewable energy sources which can meet the demand of globally increasing energy consumption. As Hydrogen Evolution Reaction (HER) needs both highly active and robust catalysts owing to their sluggish kinetics, numerous advanced researches have been reported dealing with the enhancement of catalytic properties. Herein, we present rhodium based ternary sulfide hollow nanostructure via synthesizing core-shell nanoparticles with the difference of decomposition temperature of precursors followed by post-treatment such as etching step. Due to their compositional and structural properties, rhodium based ternary sulfide hollow nanostructure exhibits highly enhanced catalytic activity and stability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-515**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Seed-mediated synthesis of rhombic dodecahedral PtCu@Ru nanoparticles

남경식 박종식 이광렬*

고려대학교 화학과

Seed-mediated synthesis method is receiving a great attention as a facile synthetic route to structurally well-defined nanocrystals, which determine the surface energy and stability of nanocrystals. Herein, we report a seed-mediated synthesis of a hollow PtCu@Ru nanocages, which involves the preparation of PtCu seed and subsequent deposition of Ru shell on it. Also, this Ru-based alloy nanostructure gives enhanced electrocatalytic activity toward oxygen evolution reaction in alkaline media.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-516**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Heavy metal ion removal using Bur-like iron oxide nanocapsules

진예진 전효경[1] 이하진[1,*]

이화여자대학교 화학나노과학과 [1]한국기초과학지원연구원 서울서부센터

Bur-like iron oxide nanocapsules (IO-NCs)with or without polymer core were synthesized by controlled heat treatment of the IO nanoneedle-coated polymer particles. The structure of the IO-NCs was characterized by Electron Microscopies such as FE-SEM and FE-TEM and X-ray diffractometer. The IO-NCs were applied to remove both anionic [Cr(V)] and cationic [Pb(II) and Cu(II)] heavy metal ions. The maximum removal capacities of IO-NCs without polymer core were **, **, ** mg/g for Cr(III), Pb(II), Cu(II), respectively. While, the maximum removal capacitis of IO-NCs with polymer core were **, **, ** mg/g for Cr(III), Pb(II), Cu(II), respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-517**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Neutron diffraction analysis of complex perovskite oxynitrides $AM_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$ (A = Sr, Ba; M = Li, Na) and $AMg_{0.2}Nb_{0.8}O_{2.6}N_{0.4}$

문건호 김영일[1,*]

영남대학교 에너지융합공학과 [1]영남대학교 화학과

The crystal structures of the complex perovskites, $AM_{0.2}Nb_{0.8}O_{3-x}N_x$ (A = Sr, Ba; M = Li, Na, Mg), were studied by using neutron powder diffraction. Rietveld refinement confirmed the formation of three-dimensional perovskites, as well as the stabilization of alkali cations on the octahedral sites rather than on the dodecahedral sites. In all six compounds, alkali cation and Nb^{5+} were disordered completely despite large mismatches of charge and size. The crystal symmetry of the average structure depended on the size of the dodecahedral cation: simple cubic for $BaM_{0.2}Nb_{0.8}O_{3-x}N_x$ and body-centered tetragonal for $SrM_{0.2}Nb_{0.8}O_{3-x}N_x$. This trend coincides with the symmetry transition from $BaNbO_2N$ (*Pm*-3*m*) to $SrNbO_2N$ (*I*4/*mcm*). The lattice volume increased in the order $BaLi_{0.2}Nb_{0.8}O_{2.8}N_{0.2} < BaMg_{0.2}Nb_{0.8}O_{2.6}N_{0.4} < BaNbO_2N < BaNa_{0.2}Nb_{0.8}O_{2.8}N_{0.2}$, which is the same for the Sr-compounds. Among the tetragonal Sr-compounds, tetragonal ratio, $c/\sqrt{2}a$ increase in the order, $SrNa_{0.2}Nb_{0.8}O_{2.8}N_{0.2} < SrLi_{0.2}Nb_{0.8}O_{2.8}N_{0.2} < SrNbO_2N < SrMg_{0.2}Nb_{0.8}O_{2.6}N_{0.4}$. The nitrogen in $SrM_{0.2}Nb_{0.8}O_{3-x}N_x$ (M = Li, Na, Mg) favors the axial 4a site over the equatorial 8h site. The structural variations among the present compounds will be compared with those of the Ta-analogues, $AM_{0.2}Nb_{0.8}O_{3-x}N_x$.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-518**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ionic conductivity of Li-containing defect perovskites, $Ca_{1-x}(Li_xTa_{1-x})O_{3-y}N_z$ (x = 0.08. 0.18, 0.28)

<u>박희경</u> 김영일*

영남대학교 화학과

Perovskite oxynitrides, $Ca_{1-x}(Li_xTa_{1-x})O_{3-y}N_z$ (x = 0.08, 0.18, 0.28), contain mobile Li cations within a unusual lattice that contain abundant vacancies on the dodecahedral sites and the mixed anion components of O and N. In this regard, ionic conductivity of $Ca_{0.92}(Li_{0.08}Ta_{0.92})O_2N_{0.84}$, $Ca_{0.82}(Li_{0.18}Ta_{0.82})O_{1.94}N_{0.68}$, and $Ca_{0.72}(Li_{0.28}Ta_{0.72})O_{1.88}N_{0.52}$ was studied by ac impedance spectroscopy as a function of x. The conductivity measurement was performed in H_2/H_2O atmosphere in the temperature range of 25-350℃. As revealed by the equivalent-circuit analysis, the ionic conductivity decreased with the increase of x. At 350℃, the ionic conductivities were evaluated to be $10^{-5.1}$ S/cm, $10^{-5.8}$ S/cm, and $10^{-6.5}$ S/cm for x = 0.08, 0.18, and 0.28, respectively. It is speculated that the ionic conductivity of $Ca_{1-x}(Li_xTa_{1-x})O_{3-y}N_z$ is governed by the vacancy defects on the anion lattice. $Ca_{0.72}(Li_{0.28}Ta_{0.72})O_{1.88}N_{0.52}$ contains most amount of Li, but on the other hand, it also contains most amount of anion vacancy. The results of ionic conductivity measurement implies that the latter effect dominates.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-519**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Partial nitridation and ionic conductivity of Li_4SiO_4

김한슬 김영일*

영남대학교 화학과

Tetralithium silicate, Li_4SiO_4, is one of the classical ionic conductors. This work made an attempt to modify the Li content and anion lattice of Li_4SiO_4, in view of improving the ionic conductivity. In particular, Li_2CO_3 and Si_3N_4 were mixed in a ratio of Li:Si = 5:1, and heated in NH_3 at 850℃, aiming at an oxynitride phase with a nominal formula of Li_5SiO_3N. For comparison, Li_4SiO_4 was synthesized by heating a stoichiometric mixture of Li_4SiO_4 and SiO_2 in air at 850℃. According to the powder X-ray diffraction, the oxide and oxynitride phases were isostructural with the monoclinic symmetry. Combustion analysis showed a nitrogen content of 1.34 wt. % in the oxynitride phase, which corresponds to the formula of $Li_{4.1}SiO_{3.9}N_{0.1}$. As observed from the diffuse-reflectance spectroscopy, above nitridation caused a remarkable decrease of band gap, from 5.6 eV in Li_4SiO_4 to 4.8eV $Li_{4.1}SiO_{3.9}N_{0.1}$. Ionic conductivity of Li_4SiO_4 and $Li_{4.1}SiO_{3.9}N_{0.1}$ were measured by ac impedance spectroscopy in N_2 atmosphere in the temperature range of 25-400℃. As revealed by the equivalent-circuit analysis, $Li_{4.1}SiO_{3.9}N_{0.1}$ had higher ionic conductivity than Li_4SiO_4 by an order. At 251℃, the former had an ionic conductivity of $10^{-5.2}$ S/cm, and the latter, $10^{-6.1}$ S/cm.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-520**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation and characterization of thermochromic VO_2/SiO_2 composite film

김종민 정영희[1] 심현관 김영일*

부경대학교 화학과 [1](주)애드크로 기술연구소

Monoclinic VO_2 is one of the most widely studied thermochromic materials for theenergy saving smart window. In order to be used for smart window which can beswitched in transmission of solar flux by temperature, the very stable and durable thinfilm of VO_2 must be prepared. Although there are many methods of thin filmpreparation for inorganic materials such as physical and chemical vapor deposition, themost cost-effective and commercially feasible method is wet-coating method. VO_2 hasseveral polymorphism and can be transformable to other crystal phases. It also can beeasily oxidizable to higher oxidation state. Therefore the preparation of the stablemonoclinic VO_2 film is one of the important issues for the thermochromic smartwindow.In this study we have prepared monoclinic-VO_2/SiO_2 composite thin film by wetcoatingmethod and compared with VO_2 film imbedded in polymer that is usually usedin tinting films. We synthesized monoclinic VO_2 nanoparticles firstly by hydrothermaland post-annealing method and prepared the coating solutions by the dispersion ofthe nanoparticles with a silica precursor or acrylic polymer in organic solvent. Thethermochromic characteristics and stability of the thin films of VO_2 that are preparedby bar-coating will be discussed.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-521**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Low odor, high performance and sustainable hydrocarbon resin

이상현

(주)코오롱 중앙기술원 석유화학연구그룹

1970 년 이전 원유를 나프타 크래킹하여 나온 일부 C5, C9 유분은 활용가치가 떨어져 수소화 과정을 거쳐서 연료로 사용되었다. 하지만 코오롱은 이런 C5, C9 유분을 원료로 중합 및 수소첨가 반응을 거쳐 점착부여수지를 개발하였으며, 현재 Tackifier 시장에서 국내 1 위, 세계 3 위의 생산 및 판매량을 기록하고 있다. 또한 코오롱은 이러한 유분과 나날이 공급 경쟁력이 증대되는 Shale gas 와의 공중합을 통해 새로운 Tackifier 개발에 박차를 가하고 있다. 이로써 생기는 Tackifier Sustainability, high performance 구현에 대한 실험 결과를 다루고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-522**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization of CuZn thin film deposited by RF co-sputtering method

최아롬 강유진 이석희 오설미[1] 강용철[*]

부경대학교 화학과 [1]부경대학교 공동실험실습관

In this research, the CuZn thin films were deposited by radio frequency (RF) magnetron co-sputtering method using metallic Cu and Zn targets. The deposited CuZn thin films were analyzed with a surface profiler, atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and Auger electron spectroscopy (AES). Thickness of the CuZn thin films was measured by the surface profiler and was regulated by deposition time to achieve at 200±8 nm. The morphology and root mean square (RMS) roughness of CuZn thin films were studied by AFM. The determined roughness values were in the range from ~20 to ~2 nm. The chemical environment of CuZn thin films was investigated with XPS and AES. The main Cu and Zn peaks were observed in XPS survey spectra. It implies that CuZn thin films were successfully fabricated on Si (100) substrate. The relative atomic ratio of CuZn thin films were calculated by two different methods. One is using high resolution XPS spectra (Cu 2p and Zn 2p) and the other is Auger peak-to-peak height (APPH) of AES spectra (Cu LMM and Zn LMM). Both results showed relatively similar ratios in acceptable error range.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-523**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Surface Analysis of Copper-Zinc Nanofibers Fabricated with Electrospinning Technique

최아롬 강유진 강용철*

부경대학교 화학과

Cu and Zn nanofibers (CuZn NFs) were fabricated with electrospinning technique. The CuZn/polyvinylpyrrolidone (PVP) solution was prepared with copper sulfate pentahydrate and zinc acetate dihydrate. Distilled water was used for solvent and PVP was used for regulating the viscosity of the CuZn/PVP solution. The CuZn/PVP NFs were fabricated with electrospinning technique using the CuZn/PVP solution. The average diameter of obtained CuZn/PVP NFs was measured by optical microscopy with Motic image plus 2.0 program and was determined about 600 nm. In thermogravimetric/differential thermal analysis (TG/DTA) data, the appropriate calcination temperature was determined to remove the solvent and to decompose PVP. After calcination of CuZn/PVP NFs at 353 K in ambient environment for 5 hrs, the solvent in the NFs was removed. X-ray photoelectron spectroscopy (XPS) was employed to investigate the chemical environment and the oxidation states of the synthesized CuZn/PVP NFs. The main C 1s, Cu 2p, and Zn 2p XPS peaks were observed from the XPS survey spectra. Therefore, we could conclude that the CuZn/PVP NFs were successfully fabricated. The CuZn NFs were obtained after decomposition of PVP by annealing process at 873 K in Ar atmosphere for 5 hrs. This was confirmed that the intensities of C 1s and N 1s peaks were decreased after calcination comparing with before calcination.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-524**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization of ZnSn thin films fabricated by RF co-sputtering method

이석희 강유진 최아롬 오설미[1] 강용철*

부경대학교 화학과 [1]부경대학교 공동실험실습관

Zinc tin oxide (ZTO) has been applied for various devices such as photoelectric devices, solar cells, UV sensors, and piezoelectric devices. Because ZTO has low resistivity, high transparency, appropriate optical properties, and large field-effect mobility. Before investigating the ZTO films, we fabricated the ZnSn thin films by radio frequency (RF) co-sputtering method using pure Zn and Sn metal targets. The obtained ZnSn thin films were investigated using Auger electron spectroscopy (AES), a surface profiler, X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). Thickness of the thin films was measured by a surface profiler and was found to be at 200±10 nm. Deposition rates of pure Zn and Sn thin films were determined with thickness and sputtering time for optimization. The morphology and root mean square (RMS) roughness of ZnSn thin films were studied by AFM. The chemical environment and relative atomic ratio of Zn to Sn of the fabricated ZnSn thin films were characterized with XPS and AES. From XPS survey spectra, we could conclude ZnSn thin films were successfully deposited on Si(100) substrate. The chemical environment of ZnSn thin films were investigated in detail with high resolution XPS spectra in the electron binding energy regions of Zn 2p and Sn 3d. The relative atomic ratios of Zn to Sn considering atomic sensitivity factors (ASF) were determined from the results of XPS and AES independently. Those were found to be consistent in allowed error.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-525**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Investigation of copper-tin thin films synthesized by rf magnetron co-sputtering method

강유진 강용철*

부경대학교 화학과

Copper-tin (CuSn) thin films were synthesized by radio frequency (rf) magnetron co-sputtering method with pure Cu and Sn metal targets. The rf powers on the targets were varied to adjust the ratio of Cu to Sn in CuSn thin films. CuSn thin films were characterized by a surface profiler (alpha step), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), X-ray induced Auger electron spectroscopy (XAES), and contact angle measurement. The results of surface profiler showed that the thickness of CuSn thin films was fixed at 200±10 nm, which was regulated the deposition time. Bronze structures such as Cu20Sn6 and Cu39Sn11 phases were observed from XRD spectra in co-sputtered thin films. In the survey XPS spectra, the main Cu and Sn peaks were observed. It implies that CuSn thin films were successfully synthesized on the substrate. The oxidation states and chemical environment of Cu and Sn were investigated with high resolution Cu 2p and Sn 3d XPS spectra and Cu LMM Auger spectra. The wettability of the films was studied using contact angle measurement with distilled water (DW) and ethylene glycol (EG) and then the surface free energy (SFE) was determined by contact angle data.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-526**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization and preparation of hydrogel lens using high compatible material

이민제 성아영*

대구가톨릭대학교 안경광학과

The basic ophthalmic lens with addition of N,N-dimethylacrylamide(DMA) and N-methyl-N-vinylacetamide(NMV) were manufactured. The optical and physical characteristics of ophthalmic lens were evaluated by measuring water content, refractive index and optical transmittance. The water content of sample containing Ref., DMA group and NMV group was in the average of 34.48%, 35.54 ~ 49.19% and 36.28 ~ 44.95%, respectively. And also, refractive index of the sample containing Ref., DMA group and NMV group was in the average of 1.4350, 1.4330 ~ 1.4131 and 1.4335 ~ 1.4195, respectively. Standard Hydrogel monomer containing DMA and NMV was expected to be used usefully as a material for fabricating hydrophilic functional ophthalmic lens.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-527**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Photopolymerization and characterization of hydrogel lens material

김득현 성아영*

대구가톨릭대학교 안경광학과

The functional hydrogel lens containing HEMA(2-hydroxyethylmethacrylate) were manufactured by photopolymerization. And also, the physical properties of the produced hydrogel lens were measured and analyzed. Radical cure of the HEMA monomer was facilitated by the incorporation of the photoinitiator HMP(2-hydroxy-2-methylpropiophenone) into the uncured at 0.5 wt%. Photoinduced polymerization at 254 nm was complete after 15 min. The hydrogel polymer was manufactured by using photopolymerization process and the results of physical properties showed that water content and refractive index of sample were in the range of 33.78~36.07% and 1.434~1.437, respectively. the refractive index was higher them that of thermal polymerization The produced copolymer by photopolymerization was suitable for hydrogel lens.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-528**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Zeolitic Imidazole Framework-8 (ZIF-8) nano-sheet with exfoliated metal hydroxide precursor

곽기원 김동표*

POSTECH 화학공학과

Synthesis of Metal-Organic Frameworks (MOFs) nano-sheets is studied by many researchers with various trials. Most of reported papers synthesized bulk MOF particles firstly and exfoliate the MOF with external mechanical force. These approaches are only valid for specific kinds of MOFs and the exfoliation steps need long times. The thickness of 2D nano-sheets are not uniform and the lateral size is limited to sub-micrometer size.In this report, as-synthesized zinc hydroxide layered structures are exfoliated into nano-meter scale thickness with ultra-sonication in microreactors and the exfoliated zinc hydroxide are treated with 2-methylimidazole, organic ligand which forms Zeolitic Imidazole Framework-8 (ZIF-8; a subclass of MOFs) with zinc ions, and the layered zinc oxide structures are successfully converted into ZIF-8. The thickness of MOF nano-sheets are 40 nm and the lateral size is 5 micrometers. The whole conversion of metal hydroxide into MOF is confirmed with XRD spectra analysis.These two-step microfluidic exfoliations and MOF conversion process are proceeded in one-flow microreactor and whole process time is sharply reduced compared with conventional 2D nano-sheet MOF synthesis methods. And these nano-sheets of MOFs can be utilized various toward membrane and molecular separation fields due to its porous structure and selective adsorption properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-529**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

In-situ modification of nanodiamond by one-pot design and its influence on the properties of nitrile-butadiene rubber nanocomposites

zhangyinhang 박수진[1,*]

인하대학교 화학 [1]인하대학교 화학과

3-Mercaptopropyltrimethoxysilane (MPTMS)–ethanol solution treated nitrile butadiene rubber/nanodiamond (NBR/ND) polymer nanocomposites were prefabricated in-situ by a novel environmentally friendly one-pot design. The nanodiamond (ND) and modified nanodiamond (MND) were characterized by using wide angle X-ray diffraction (WAXD), Fourier transformation infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), an adsorption analyzer (BEL BELSORP), thermal gravimetric analysisis (TGA), and X-ray photoelectron spectroscopy (XPS). The results show that the pristine ND is provided not only with high specific surface area, but also with abundant active organic groups, especially hydroxyl and carboxyl groups, which confirms the hydrophilic properties of nanodiamond. The morphology of the fracture surfaces of NBR/(M)ND nanocomposites are studied by high resolution scanning electron microscopy (HR-SEM). The dynamic rheological properties of NBR/(M)ND nanocomposites were characterized by rubber processing analyzer (RPA). The NBR/MND composites exhibited superior mechanical property attributing to the stronger interfacial interaction via covalent bonding between MND and NBR molecules compared to the NBR/ND composites that connected by weaker π-π stacking.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-530**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Birch-type hydrogenation of few-layer graphenes: products and mechanistic implications

ZHANGXU Rodney Scott Ruoff[1,*]

기초과학연구원 다차원탄소재료료연구단 [1]UNIST 화학과

The functionalization of graphene changes its physical and chemical properties. Complete hydrogenation of graphene affords graphane (CH)n, as-yet an unreported material predicted to have a large band-gap.1 When hydrogenation is substoichiometric, DFT calculations predict the formation of domains exhibiting ferromagnetism over certain temperature ranges2. We show here that well-defined graphenes of varying thickness can be efficiently hydrogenated using a Birch-type reduction3-5. Mechanically-exfoliated as well as CVD-grown bi- and multilayer graphene can be hydrogenated by using Li as the reducing reagent and H2O as the proton donor; the hydrogenation of multilayer samples occurs to a less extent than in monolayers. The present hydrogenated graphenes undergo dehydrogenation upon thermal annealing, with a process that is most facile for reduced monolayers. Methanol is a weaker proton donor in the Birch-type reduction, especially when bi- and multilayer graphenes are hydrogenated. Reactivity under the Birch conditions is independent of stacking orientation: CVD-grown AB-stacked graphene has a similar reactivity to 'mis-oriented' bilayer graphene. Raman mapping indicates that hydrogenation proceeds from the edge to the center of bilayer graphene, a result that implicates that the intercalation of Li and/or protons between graphene layers may play a role. This work was supported by IBS-R019-D1.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-531**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of mercapto-terminated silane treatment on rheological behavior of rice bran carbon-reinforced nitrile butadiene rubber composites

zhangyinhang 박수진[1,*]

인하대학교 화학 [1]인하대학교 화학과

The surface morphology and structure of novel rice bran carbon (RBC) were characterized by X-ray diffraction, thermogravimetric analysis, high-resolution scanning electron microscopy (HR-SEM), Raman spectroscopy, and adsorption analysis. The RBC/nitrile butadiene rubber (NBR) polymer-matrix composites were fabricated by using the latex compounding technique, based on the superior hydrophilic characteristics of RBC. The covalent bonding process was conducted by in situ interfacial modification technique. The dispersion of RBC and the interfacial morphologies between the RBC and NBR matrix were confirmed by HR-SEM. The bonding mechanism was analyzed in detail by mechanical and dynamic rheological determinations. At the same filler concentration, the MPTMS treated composites exhibited stronger mechanical properties than original RBC/NBR composites, as the interfacial interaction via MPTMS connected RBC and NBR molecules was stronger than the interaction in NBR/RBC composites connected by hydrogen bonds and weaker π-π stacking.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-532**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Thermoregulatory liquid-liquid extraction for fabricating nanodiamond nanocluster decorated-graphene oxide/epoxy nanocomposites

zhangyinhang 박수진[1,*]

인하대학교 화학 [1]인하대학교 화학과

Hybrid fillers composed of nanodiamond (ND) decorated graphene oxide (GO) were incorporated into epoxy matrix with a novel thermoregulatory liquid-liquid extraction method. Energy dispersive spectroscopy, X-ray diffraction spectroscopy, Fourier transform infrared and X-ray photoelectron spectroscopy analysis confirmed chemical bonding between the 3-aminopropyltriethoxysilane functionilizatied nanodiamond (ND-APTES) and 3-Glycidoxypropyltrimethoxy silane functionalized graphene oxide (GO-GMPTS). The morphology of the hybrid filler, GN was characterized by high-resolution transmission electron microscopy. ND nanoclusters with an average diameter of 50-100nm were uniformally grown on the GO surface. The hybrid filler provided significant enhancement of mechanical properties, such as flexural strength, flexural modulus and impact strength. In particular, the epoxy composites containing 0.1wt% hybrid GN exhibited a higher mechanical behavior compared to the one containing 0.2 wt% GO.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-533**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Induced Dipole in Vanadium-doped Zinc Oxide Nanosheets and its Effects on Photoelectrochemical Water Splitting

이송미 이민형[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Appropriate control of band bending at the interface between semiconductors and electrolytes are deeply related to the performance of photoelectrochemical (PEC) water splitting. Dipole formed at near surface of semiconductors can control directions of band bending at the interface. Charged molecule coating and piezoelectric materials applied on PEC electrodes have been demonstrated band bending control depending on the dipoles inside. However, chemical and piezoelectric approaches have demerit of chemical instability and temporary dipole induce. To overcome the problems, we applied ferroelectric materials that can induce spontaneous dipoles on PEC water splitting. Ferroelectric ZnO nanosheets (NSs) were synthesized by in-situ doping of vanadium (V) in ZnO during hydrothermal process. The dipole effect on performance of V-doped ZnO PEC for water oxidation was systematically investigated under controlled dipole directions. Consequently, positively polarized V-doped ZnO photoanodes exhibit enhanced water splitting efficiency compared to negatively polarized ones due to favorable band bending for carrier transport from semiconductor to water

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-534**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Antimicrobial Property and XPS Analysis of Copper-Tin Thin Films

강유진 김동우 김학준 강용철*

부경대학교 화학과

Copper-tin (CuSn) thin films were fabricated by radio frequency (RF) magnetron co-sputtering method onto Si substrate. Pure Cu and Sn metal targets were used and the RF powers were adjusted for obtaining CuSn thin films with desired relative atomic ratio of Sn to Cu. CuSn thin films were characterized by a surface profiler (alpha step), X-ray photoelectron spectroscopy (XPS), and antimicrobial test. The thickness of CuSn thin films was controlled about 200±10 nm by regulating deposition time. Brfore the antimicrobial test, the relative atomic ratio of Cu and Sn was determined by high resolution XPS spectra considering atomic sensitivity factors (ASF) of the elements. The oxidation states of CuSn thin films and the chemical environment of the films after antimicrobial test were analyzed with high resolution XPS spectra in regions of Cu 2p and Sn 3d. An antimicrobial activity against *Staphylococcus aureus* (*S. aureus*) was evaluated at different contact times between CuSn films and bacteria suspension. The results of antimicrobial test showed that co-sputtered thin films (CuSn) exihibited higher antimicrobial efficiency than mono-sputtered thin films (Cu or Sn).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-535**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Antibacterial activity of CuSn thin films deposited with various RF powers

강유진 김동우 김학준 오설미[1] 강용철*

부경대학교 화학과 [1]부경대학교 공동실험실습관

CuSn thin films were deposited by radio frequency (RF) magnetron co-sputtering method with pure Cu and Sn metal targets and at various RF powers. The co-sputtering process was performed in different rf powers and sputtering times to manipulate the thickness of CuSn thin films and relative atomic ratio of Cu/Sn. CuSn thin films were investigated with a surface profiler (alpha step), X-ray diffraction (XRD), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and antibacterial test. Thickness of CuSn thin films was fixed at 200±10 nm. Bronze structure like $Cu_{20}Sn_6$ phase was observed in co-sputtered thin films after sterilization process. The morphology of the deposited CuSn thin films was studied with AFM images. The oxidation states Cu and Sn in CuSn thin films and the chemical environment of films after antibacterial test were investigated with high resolution Cu 2p and Sn 3d XPS spectra. An antibacterial activity against *Escherichia coli* (*E. coli*) was monitored at various contact times between CuSn films and bacteria suspension.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-536**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Various Types of Hierarchically Oxidized Morphologies and Their Comparison Studies for Efficient Oil/Water Separation

임용택 최원산*

한밭대학교 화학생명공학과

Due to the frequent oil spill accidents, the increasing industrial oily wastewater and attention to the preservation of the environment, there is an increasing and urgent need to develop novel materials or techniques which can separate the water from the oil/water mixture effectively and quickly. The development of low cost materials with chemically and physically stable properties has become a challenging task for oil/water separation and related applications. Various materials such as sponges, meshes, filter papers, and fabrics have been proposed for oil/water separation. Among them, metal meshes have been considered as the most suitable templates due to their characteristics of low cost, high porosity, and good liquid permeability. However, very toxic chemicals are generally used for oxidation of metal meshes. We report a facile green approach for preparing hierarchically oxidized metal meshes. A facile heat treatment method suggested by our group was compared with previously reported chemical methods. The resulting our meshes exhibited a significant potential for highly efficient oil/water separation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-537**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Instant and Fast Removal of Heavy Metal Ions using Tea-Baglike Adsorbents

배지영 최원산*

한밭대학교 화학생명공학과

Humans are being exposed through contaminated water, coal combustion, paints, industrial process from product manufacturing. Heavy metal ions have direct adverse effects on human health and the environment when they are illegally discharged. Cases of serious side effects have been reported since they are accumulated in the human body along the food chain. Because of effectiveness of adsorption process, numerous adsorbents have been proposed for efficient removal of heavy metal ions or organic pollutants in waste water. However, previously reported adsorbents and adsorption process are not suitable for small scale enterprise and individual user. Development of a portable heavy metal ion remover which can be used even by untrained user is highly demanded. Sponge is portable, easy to use, and ubiquitous materials. Polymer brushes possess advantages of numerous reaction sites and pH-responsive behaviors for control of adsorption/desorption. Thus, highly porous sponge composites decorated with polymer brushes via “grafting-from” or “grafting-to” polymerization was developed for fast and efficient removal of heavy metal ions in waste water or drinkable water.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-538**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Palladium-2D Hybrid Nanomaterials Hybrids for Highly Efficient Visible-Light Responsive Photocatalyst

신현호 강은미[1] 이아름[2] 임동권[3,*]

고려대학교 KU-KIST융합대학원 [1]고려대학교 NBIT [2]고려대학교 KU-KIST 융합대학원 / NBIT [3]고려대학교 KU-KIST 융합대학원

Two dimensional (2D) materials such as molybddenum disulfide (MoS2), tungsten disulfide (WS2), tungsten diselenide (WSe2) and reduced graphene oxide (rGO) have recently attracted scientific attentions because of their various applications in catalysis, energy devices, etc. Here, we report palladium nanodot and 2D hybrid nanomaterials as a highly efficient visible-light responsive photocatalyst for Suzuki-Miyaura coupling reaction. The presence of 2D materials was found to be greatly helpful in expediting the C-C coupling reaction because of the unique band gap structures which can absorb visible light. In this poster, we are going to provide the detailed experimental parameters and results that performed to unveil the underlying mechanism of enhanced photocatalytic activity of Pd-2D hybrid nanomaterials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-539**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Bifunctional devices with Amphiprotic Property for Oil/Water Separation and Pollutant Purification

한나라 최원산*

한밭대학교 화학생명공학과

Marine ecosystem has suffered from severe environmental damage because of the frequent oil spillage and oily pollutant discharge. Senseless discharge of aqueous toxic pollutants from industry has also emerged as a serious problem in recent years. To deal with the problems, various methods involving sol-gel, chemical etching, self-assembly, hydrothermal, and electrospinning have been proposed. However, these methods are normally used for individual issue only. Few studies have provided a solution for satisfying both issues and these studies have focused on decomposing organic pollutants in water using catalysts. Herein, we report a combined device for addressing both issues.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-540**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Hierarchical Surface Design of Catalysts for Chemical Buffer layers and Fast Reactions

강병권 최원산[1,*]

한밭대학교 응용화학과 [1]한밭대학교 화학생명공학과

Structural design of nanocatalysts has been proven to be the most effective method to enhance their catalytic activity and stability. Considerable attention has been devoted to dispersing nanocatalysts onto matrices to improve the stability and activity of nanocatalysts. Direct design for surface structures of nanocatalysts has been considered to tune the physicochemical properties of nanocatalysts. In our previous study, we demonstrated that needlelike and less reactive surfaces of catalysts could be one of good surface designs to enhance the stability and activity of catalysts. Herein, we report optimized surface design of heterogeneous catalysts based on polyelectrolyte brushes as cilia and polymer particles as catalyst supports.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-541**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A Highly Active Palladium Catalyst for Suzuki Coupling Reaction with Reduced Graphene Oxide Coated Gold Nanorods

강은미 임동권[1,*]

고려대학교 NBIT [1]고려대학교 KU-KIST 융합대학원

The Suzuki coupling reaction which is the coupling of an organoboron reagent and an organic halide in the presence of a palladium catalyst and base is a powerful one step pathway of catalytic C-C bond formation. Also, the efficient use of solar energy has been widely investigated for increasing energy and environmental issues. The plasmonic Gold nanorods (AuNRs) have large extinction cross sections and wavelengths covering the entire solar spectrum. Wang et al. reported on the direct harvesting of visible-to-near-infrared light for chemical reactions by use of plasmonic Au-Pd nanorods. Graphene is a monolayer of carbon atoms packed into a two-dimensional (2D) hexagonal structure, which is a special material with excellent photothermal property. We studied reduced graphene-coated AuNRs which were integrated with catalytic Pd nanoparticles through seeded growth. The Suzuki coupling reaction with Iodobenzene and Phenylboronic acid was used to examine the reaction. We used Xe lamp for matching solar spectrum and controled temperature and light for comparing photocatalytic and photothermal effects. We demonstrated that the Suzuki coupling reaction is promoted and improved due to plasmonic photocatalysis and photothermal conversion.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-542**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Influence on Mechanical Properties of Epoxy Composites with Graphene Oxide from Pitch-based Carbon Fibers

김명석 박수진*

인하대학교 화학과

In this study, effect on fracture toughness of epoxy reinforced composites with graphene oxide from pitch-based carbon fibers (pGO) was investigated. Chemical exfoliation of pitch based carbon fiber (pCF) by typical modified Hummers method is attempted to provide pGO. The contents of pGO into epoxy resin were improved their fracture toughness property. An impressive fracture toughening effect is observed with less than 0.1 wt% pGO. A maximum in toughness at loadings as small as 0.02 wt% is observed for all contents of pGO. A microcrack mechanism is proposed based on microscopy of the fracture form. Due to the stress concentration by pGOs, microcracks may be formed to absorb the fracture energy. However, above a certain pGO concentration, the coalescence of microcracks appears to facilitate crack propagation, lowering the fracture toughness.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-543**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of Silicon Carbide Contents in Thermal Stabilities and Mechanical Properties of Pitch-carbonized Glass Fibers-reinforced Composites

김명석 박수진*

인하대학교 화학과

In this work, the effect of SiC contents was investigated in thermal stabilities and mechanical interfacial properties of pitch-carbonized glass fibers-reinforced composites. Mechanical properties of the composites were studied using interlaminar shear strength (ILSS) and critical stress intensity factor (K1c) measurements. The cross-section morphologies of pitch-carbonized glass fibers-reinforced composites were observed by scanning electron microscope (SEM). Also, the surface properties of basalt fibers were determined by Fourier transform infrared spectroscopy (FT-IR). The thermal stabilities of the carbon fibers-reinforced composites were investigated by thermogravimetric analysis (TGA). And thermal conductivity was studied by flash diffusivity analyzer (LFA). From the results, these composites were explained that suitable amount of silicon carbide (SiC) played an important role in improving thermal conductivity and mechanical interfacial properties.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-544**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect on activated carbons of surface functional groups and charge/discharge cycle behaviors for methane storage

김명석 박수진*

인하대학교 화학과

The effect on methane storage of activated AC surface functional groups behavior and cycling properties were investigated. Chemical activation process was conducted by treatment with KOH. Structural properties were evaluated by X-ray diffraction (XRD) and morphology properties were studied by scanning electron microscopy (SEM) and transmission electron microscope (TEM). Textural properties and microporosity were determined from N2/77 K adsorption-desorption isotherms using the Brunauer-Emmett-Teller (BET) equation and the Horvath-Kawazoe (HK) method. Surface functional groups were indicated by Fourier-transform infrared spectroscopy (FT-IR) and were made clear functional groups by X-ray photoelectron spectroscopy (XPS). Methane storage capacity and cycling properties were conducted by using methane storage instrument at 298 K and 35 bar.In this paper, the functional group of the activated carbon surface were investigated the effects of methane storage capacities. Also, the activated carbon was performed charge and discharge cycle experiment methane storage.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-545**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

MULTI-SHELLED METAL-ORGANIC FRAMEWORK HOLLOW SPHERES BY DROPLETS LAYER-BY-LAYER ASSEMBLY

정관영 김동표*

POSTECH 화학공학과

Integrated progress has been made in the preparation and application of metal-organic frameworks (MOFs) hollow micro-/ nanostructures during the past decade. However, formation of multi-shelled metal-organic framework hollow spheres have not been reported comprehensively in the literature. Herein, we reported the MOFs coating strategy by droplets layer-by-layer assembly on the functional supports. Two kinds of MOFs with different ligands (benzenedicarboxylate or BDC and 2-methylimidazole or 2-MIM) were epitaxially and alternately grown on the functional supports, and then BDC based MOFs were selectively removed by chemical etching process. Obtained multi-shelled MOFs hollow spheres were tested by functionalization of different catalysts that were serially functionalized inner- and outer- MOF shells, showing the cascade transformation of two step fructose to 2,5-dimethylfuran by tandem catalysis. Finally, multi-shelled MOFs hollow spheres were pyrolyzed to fabricate the corresponding multi-shelled metal oxide hollow spheres, showing excellent high-capacity electrodes for lithium ion battery.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-546**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The Influence of Heat Treatment in Orthogonal Lithography on OLED Layers

채승근 이동준 정병준*

서울시립대학교 신소재공학과

For the high resolution organic light emitting diode (OLED) display, several pixel patterning technologies have been researched. Orthogonal lithography using fluorinated photoresist materials and fluorous solvents is one of challenged candidates. Soft baking and post exposure baking (PEB) in the photolithography are necessary to form a clear patterned image. The photoresist materials are removed after the lithography process. In this work, we will report the effect of OLED performance as soft baking and post exposure baking (PEB) on a hole transporting layer which is coated with a fluorinated photoresist and developed by a fluorous solvent.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-547**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The optical behavior around the phase transition of VO_2 film depends on the morphology and preferred growing axis

이명순 김 돈[*]

부경대학교 화학과

We have prepared a smart VO_2 film on a sapphire (0001) substrate by a direct thermal treat of a mixture of polyvinylpyrrolidone and $VOCl_2$ solution at 803 K under an inert condition. The optical characteristics of the film near the phase transition temperature could be controlled by the VO_2 film morphology and crystal structure. The morphology and crystal structure depend on mainly the thickness of the VO_2 film. The optical properties of the films could be grouped by three types: S, M and L-type. The S-type film, a brown colored thin film (~0.3 um in thickness), which consists of small VO_2 particles (~0.7 um in thickness) did not cut off more IR at high-T than low-T phase.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-548**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Selective determination of 5-HT and DA in presence of Ascorbic acid on Pt nanoparticles -MWCNT modified disc graphite electrode

이명순 김 돈*

부경대학교 화학과

This work describes a synthesis of platinum nanoparitcles on multi-walled carbon nanotubes (PtNPs-MWCNTs) by thermal decomposition and their study based on Raman, XRD, TEM and HR-TEM. The direct thermal decomposition synthesis was carried out using platinum precursor and could produced uniform Pt NPs with diameter of 5 nm on the surfaces of MWCNTs. The PtNPs-MWCNTs were applied as prepared, on the surface of a disc graphite electrode, showing excellent electrochemical response in the simultaneous determination of serotonin (5-hydroxytryptamine or 5-HT) and dopamine in presence of ascorbic acid. The detection limits for the two analytes were 20 nmol L^{-1} and 5 nmol L^{-1}, respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-549**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

SYNTHESIS AND STRUCTURE OF CLUSTER RHENIUM SULFITE MOLECULAR COMPLEXES AS NEW MATERIALS

LYTHIGIANG 김성진[1,*]

이화여자대학교 자연과학대학화학나노과학과 [1]이화여자대학교 화학과

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.

Octahedral rhenium cluster core $Na_{10}[Re_6Se_8(SO_3)_6]$ $Na_{10}[Re_6Se_8(SO_3)_6]$

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-550**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The effect of graphene oxide (GO) size and functional group on the mechanical properties of CNT fiber

김영진 김영관[1,*]

전북대학교 융합소재공학과 [1]한국과학기술연구원(KIST) 복합재료기술연구소 탄소융합소재연구센터

Carbon nanotubes (CNTs) has recently received a great attention due to their fascinating physicochemical properties such as lightness, chemical inertness, high electrical conductivity and mechanical strength. However, their macroscopic assembled structures (fiber, films and etc.) present a lower mechanical strength than individual CNTs because of their low packing density and poor alignment in assembled structures. Especially, the low density and poor alignment in CNT fibers result in deficient load transfer between individual CNTs and thus many efforts have been devoted to improve load transfer between individual CNTs. In this study, we utilized graphene oxide (GO) derivatives as an interlocking agent for improvement of the load transfer between individual CNTs in CNT fiber. The GO was size-fractionalized, functionalized and incorporated into CNT fibers to investigate the effect of GO size and functional groups on the mechanical properties of CNT fibers. The structures and mechanical properties of GO-incorporated CNT fibers were thoroughly characterized by using scanning electron microscopy (SEM), Favimat, Raman and X-ray photoelectron spectroscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-551**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fabrication of carbon nitride/carbon dots composites for photocatalytic degradation behaviors of rhodamine B

장익범 박수진[1,*]

인하대학교 화학화학공학융합대학원/화학 [1]인하대학교 화학과

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.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-552**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

High Efficiency and Flexible Luminescent Solar Concentrator (LSC) for Large Area Solar Windows Enabled by Massive Stokes-Shift Nanocluster Phosphors

nguyenthixuandieu 김성진[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과

Conversion of the incident solar spectrum to monochromatic light would greatly increase the efficiency of solar cells. Down conversion was suggested in the late 1970s to be used in so-called luminescent solar concentrators (LSC), also referred to as fluorescent concentrators. LSCs consist of a highly transparent plastic, in which luminescent species, originally organic dye molecules, are dispersed. These dyes absorb incident light and isotropically emit it at a red-shifted wavelength, with high quantum efficiency. Internal reflection ensures collection of part of the emitted light in the solar cells at the side(s) of the plastic body. To ensure near-unity conversion efficiency, the energy of the emitted photons ideally is only somewhat larger than the band gap of the attached solar cells and luminescent species should have a large Stoke-shift to reduce re-absorption lost.We have designed and fabricated novel luminescent solar concentrators devices composed of phosphorescent metal halide nanocluster blends with the highest power efficiency of 4.75 ±0.05%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-553**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Investigating the Roles of Fe-N_x and Fe-Fe_3C@C Species in Fe-N/C Oxygen Reduction Electrocatalysts

김재형 사영진[1] 주상훈[*]

UNIST 에너지화학공학부 [1]UNIST 화학과

Iron and nitrogen co-doped carbons (Fe-N/C) have emerged as promising non-precious metal catalysts for replacing Pt-based catalysts for oxygen reduction reaction (ORR). While Fe-N_x sites have been widely accepted as active sites for Fe-N/C catalysts, very recently, iron and/or iron carbide encased with carbon shells (Fe-Fe_3C@C) has been suggested as a new active site for the ORR. However, most of synthetic routes to Fe-N/C catalysts involve high-temperature pyrolysis, which unavoidably yield both Fe-N_x and Fe-Fe_3C@C species, hampering the identification of exclusive role of each species. In this work, in order to establish the respective roles of Fe-N_x and Fe-Fe_3C@C sites we rationally designed new model catalysts via phase conversion method from Fe_3O_4 nanoparticles supported on carbon nanotubes. It was revealed that Fe-N_x sites dominantly catalyze the ORR with 4-electron pathway, exerting a major role for the high ORR performance, whereas Fe-Fe_3C@C sites mainly promote 2-electron reduction of oxygen and sequential peroxide reduction (2 × 2 oxygen reduction), playing an auxiliary role for the ORR.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-554**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Synergistic Effect of Photothermal and Chemotherapy using Camptothecin Functionalized Gold Nanorods

양수정 정선도[1] 박명환[1,*]

삼육대학교 화학과 [1]삼육대학교 화학과

Chemotherapy is a major therapeutic approach for the treatment of cancers, but nonspecific delivery of drugs leads to normal tissues toxicities. Photothermal therapy using near-infrared(NIR) has attracted in recent years because harmless NIR minimally absorbed by skin and tissues, it can penetrate more deeply. However most photothermal agents can not provide an efficient heat transfer to cancer cells. Combining treatments with photothermal and chemotherapy is desirable to improve these problems and enhance the therapeutic efficacy. Here, we designed a NIR light-sensitive new biomaterial to achieve a synergized photothermal-chemotherapy of cancers. The camptothecin functionalized gold nonorods were fabricated through one-step place exchange reactions from cetyltrimethylammonium bromide(CTAB) gold nanorods. These materials can strongly absorb NIR light(808nm) and convert it into cytotoxic localized-heat, which accelerates release of drugs at elevated temperature. This combination of photothermal and chemotherapy has been proved to be more effective than respective monotherapies. The structural formation was characterized using ultraviolet-visible(UV) spectroscopy, Fourier transform infrared(FT-IR) spectroscopy and dynamic light scattering(DLS) spectroscopy. The release behavior of drugs induced by exposing NIR was analyzed by fluorescence spectroscopy.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-555**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of BiOClx/BiOBry/BiOIz composites nanofibers for visible-light photocatalytic investigation

장익범 박수진[1,*]

인하대학교 화학화학공학융합대학원/화학 [1]인하대학교 화학과

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.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-556**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of an environmental microfluidic chip using a colorimetric sensor

김영윤 양유열 정광윤 김장군[1] 박명환*

삼육대학교 화학과 [1]삼육대학교 소프트웨어학과

The need for rapid, sensitive, and portable identification devices for environmental toxicants have been enormous due to the increase of individual's interest in personal health care and strict governmental demand for environmental policies. Here, we have developed a simple microfluidic chip for colorimetric sensing for a wide range of harmful chemicals such as heavy metal ions and environmental toxicants. The microfluidic chip consists of 3D structured PDMS channels, silica particles and an array of fluorescent probes. Pillars in PDMS microfluidic channels generated micro-vortex instead of lamellar flowing. Three-dimensional corrugated surfaces with high surface density induced by immobilization of silica particles enhance efficient interaction between probes and analytes. Fluorescent probes provide colorimetric signals via RGB color pattern changes by interacting of various analytes. Initially, the use of porphyrin series with our microfluidic chips will be studied as a fluorescent probe for heavy metal ions. Furthermore, RGB color pattern change by metal ion binding will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-557**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mesostructured Pt-Based Bimetallic Nanospheres Containing an Intermetallic Phase as Ultrastable Self-Supported Oxygen Reduction Electrocatalysts

김호영 사영진[1] 주상훈[2,*]

UNIST 에너지및화학공학부 [1]UNIST 화학과 [2]UNIST 에너지화학공학부

Developing highly active and stable cathode catalysts is of pivotal importance for proton exchange membrane fuel cells (PEMFCs). While carbon-supported Pt-based catalysts have so far been the most active cathode catalysts, their durability and single-cell performance are yet to be improved. Herein, we report self-supported mesostructured Pt-based bimetallic (Meso-PtM; M = Ni, Fe, Co, Cu) nanospheres containing an intermetallic phase, combining the beneficial effects of transition metals (M), an intermetallic phase, a 3D interconnected framework, and a mesoporous structure. Meso-PtM nanospheres showed enhanced ORR activity, compared to Pt black and Pt/C catalysts. Notably, Meso-PtNi containing an intermetallic phase exhibited ultrahigh stability, showing enhanced ORR activity even after 50,000 potential cycles, whereas Pt black and Pt/C underwent dramatic degradation. Importantly, Meso-PtNi with an intermetallic phase also demonstrated superior activity and durability when used in a PEMFC single-cell, with record-high initial mass and specific activities.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-558**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of Graphene Oxide/BiOCl composites nanofibers and their application in photocatalytic degradation of RhB

장익범 박수진[1,*]

인하대학교 화학화학공학융합대학원/화학 [1]인하대학교 화학과

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.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-559**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Multiplexed Wide-Field Raman Bio-Imaging of Surface Roughness-Controlled Nanobridged Nanogap Particles

김종우 남상환[1] 김남훈[2] 서영덕*

한국화학연구원 나노라만융합연구센터 [1]한국화학연구원 나노바이오융합연구센터 [2]한국화학연구원 나노바이오융합연구단

Plasmonic nanostructures has been widely studied because of their various properties dependent on their size, shape, composition, and assembled structure. We employed gold surface roughness-controlled nanobridge nanogap particles (Au-RNNPs) that have stronger nanogap-enhanced Raman scattering signals, which are attributed to their enhanced electromagnetic field due to increased surface roughness. We demonstrated multiplexed Raman bio-imaging of high speed and high resolution by using custom-built wide-field Raman imaging system with Au-RNNPs. In addition, we found that Au-RNNPs are compatible with five different Raman dyes. Our results provide strategies for detection and imaging with Raman nanoprobes for optical and biomedical applications.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-560**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Chemical route strategies for VO_2 coated TiO_2 powder and their characteristics

eadi sunil babu 김성진[1,*]

금오공과대학교 신소재공학부 [1]금오공과대학교 신소재시스템공학부

Vanadium dioxide (VO_2), a well-studied thermochromic material, can undergo a reversible transition between a monoclinic phase and a tetragonal phase at a critical temperature (Tc) of approximately 68.1°C. Due to its interesting temperature-dependent optical and electrical properties induced by reversible phase transformation, VO_2 best suits as a promising material for applications such as thermochromic pigments,thermal sensors, smart IR optical windows.In this study, we prepared the VO_2 and VO_2 coated TiO_2 powders for the potential application for thermochromic smart coating glass. The VO_2 powder was prepared by V_2O_5 and Oxalic acid as the chemical precursors. The growth of VO_2 on TiO_2 nanoparticles was done by a hydrothermal method. The VO_2 and VO_2 coated TiO_2 powders were being characterized by means of X-ray diffraction, Transmission electron microscopy, Scanning electron microscopy. The powders were studied for temperature-dependent optical properties for the smart window applications.

Acknowledgment
This work was supported by the Research Funding by Kumoh National Institute of Technology. We would like to acknowledge and thank for the funding of Project – 10063553 partially supported by MOTIE in 2016.

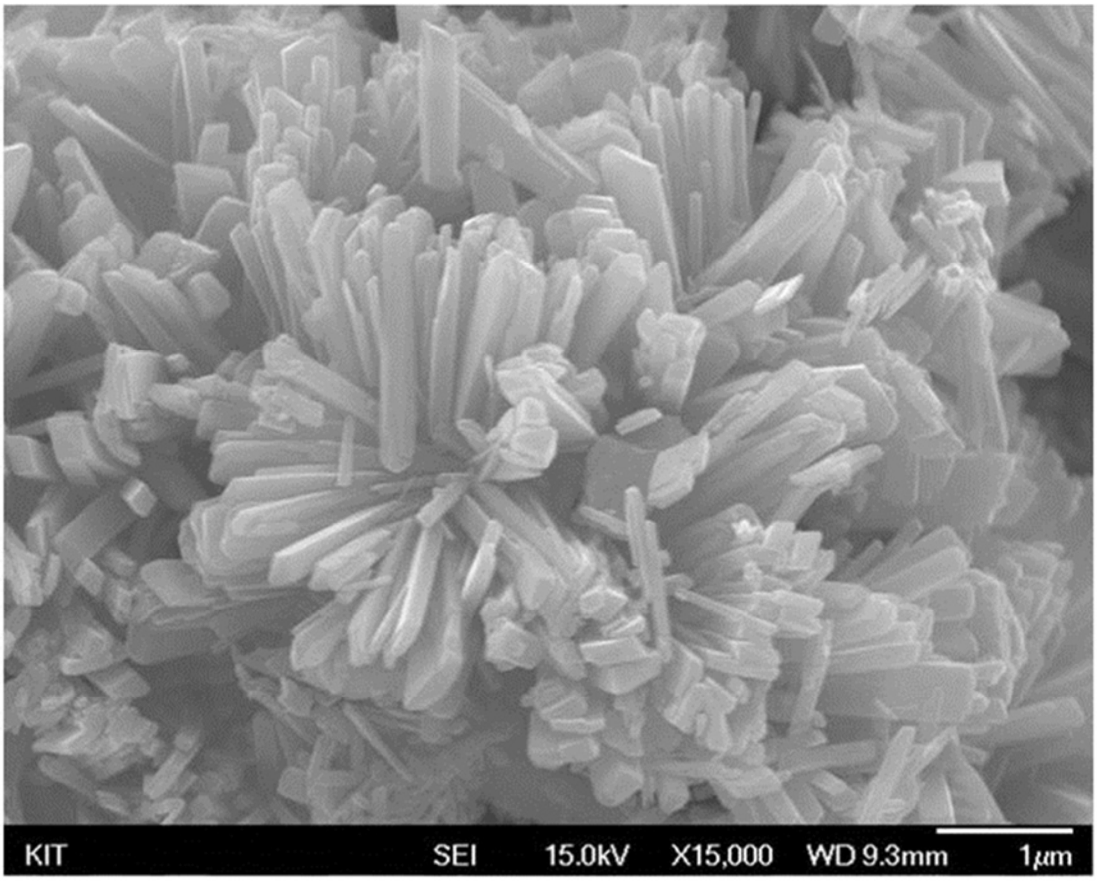


Figure shows FESEM image of VO_2 nanorods

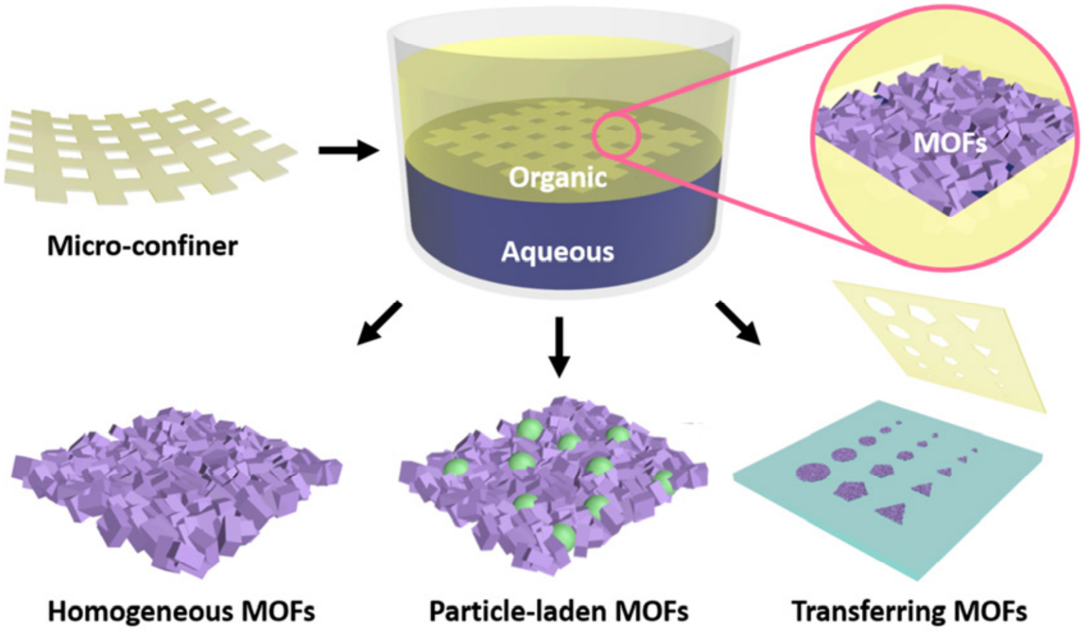
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-561**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Direct fabrication of free-standing MOF superstructures with desired shapes via micro-confined interfacial synthesis

김진오 김동표[1,*]

POSTECH 미세유체응용화학연구단/화학공학과 [1]POSTECH 화학공학과

Metal organic frameworks (MOFs) are an emerging class of multifunctional porous materials. Recently, intensive research efforts are focused on controlling the morphology on the desired substrates by improving the processability with facile functionalization in a facile and simple manner. Therefore, it is highly desirable to develop an innovative synthetic method that localizes such coordination reactions within a confined space for structuring the MOF assemblies such as films, membranes or patterns. Furthermore, the transfer of the prepared MOF features definitely facilitates the integration of MOFs into device fabrication. Herein, we develop a micro-confined interfacial synthesis (MIS) approach for fabrication of a variety of free-standing MOF superstructures with desired shapes. This approach for engineering MOFs provides three key features: (i) in-situ synthesis of various free-standing MOF superstructures with control over shape and thickness with the help of a mold membrane; (ii) assigning functionality into heterogeneous MOF superstructures by loading iron oxide nanoparticles (Fe3O4 NPs); (iii) transferring the synthesized MOF superstructural array to any desired location on flat or curved surface of various substrates. The availability of the MIS route opens the door for a number of new perspectives for fascinating device fabrication.


Micro-confiner
Organic
Aqueous
MOFs
Homogeneous MOFs
Particle-laden MOFs
Transferring MOFs

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-562**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The Enhancement of Electrocatalytic Oxygen Evolution Activity of Layered Double Hydroxide via incorporating with Exfoliated RuO_2 Nanosheet

<u>권남희</u> JINXIAOYAN 황성주*

이화여자대학교 화학·나노과학과

A remarkable enhancement of the electrocatalyst performance of Ni-Co-layered double hydroxide (Ni-Co-LDH) for oxygen evolution reaction (OER) is achieved by adapting exfoliated RuO_2 nanosheet as an additive. Even though Ni-Co-LDH is composed of high electrochemically active elements (Ni and Co), it still suffers from insufficient electrical conductivity as an efficient electrode material. To circumvent this drawback of LDH, a small amount of conductive exfoliated RuO_2 nanosheet is hybridized with Ni-Co-LDH to improve its electrocatalytic activity. Ni-Co-LDH-RuO_2 nanocomposites can be synthesized by the electrostatically-driven self-assembling between exfoliated RuO_2 nanosheet and Ni-Co-LDH nanosheet. The obtained nanocomposites show much better performances with much smaller overpotentials than does the pristine Ni-Co-LDH. The incorporation of only 1wt% RuO_2 nanosheet leads to the remarkable reduction of overpotential even similar with that of Ir/C. Such a huge drop of potential is attributable to the enlarged electrochemically active surface area and facilitated charge transfer. The present results demonstrate that exfoliated RuO_2 nanosheet can be used as an efficient additive for enhancing the electrocatalytic activity of LDH materials.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-563**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Foldamer Supramolecular Architectures via Coordination Driven Assembly of Helical *β*-Peptide Foldamers

유성현 이희승*

KAIST 화학과

Enzymes exhibit high catalytic efficiencies and substrate specificities resulting from their topological and functional complexity in the catalytic cavity. This observation has inspired chemists to mimic the supramolecular functional systems from various scaffolds such as peptide amphiphiles, synthetic hosts and non-natural folded oligomers (i.e. foldamers). Our group have reported the foldamer-based mircrostructures, termed foldectures, via solvophobic driven self-assembly of β-peptide foldamers. However, the design and synthesis of foldamer-based supramolecular system which guided and constructed through coordination bond remain significant challenge. Here, we report foldamer microstructures by coordination driven assembly of helical β-peptide foldamers and metal precursors. The hexamer of *trans*-(S,S)-2-aminocyclopentanecarboxylic acid was synthesized as coordinative foldamer ligand. The ligand exhibit stable helical conformation in both solid and solution state as expected. Foldamer based microstructures were formed from metal mediated assembly of the ligand and copper nitrate, zinc nitrate.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-564**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Powder X-ray Diffraction Analysis of Self-assembled Structures Consisted with Beta-peptide Foldamers

공진택 이희승*

KAIST 화학과

Well-designed beta-peptide foldamer is able to self-assemble to make various well-defined 3D architectures in aquous solution, named “foldecture”. The term, foldecture is coined with the compound word of foldamer and architecture. Our group have reported several unprecedented shapes of foldectures such as windmill shape and molar tooth shape, which was highly homogenous in both of size and morphology. Furthermore, in order to explore potentialities for functional materials, we recently published the study about the exposing carboxyl group to the specific rhombic facets of foldecture. We found new potential abilities of foldecture in the mechanical properties as well, such as anisotropic shape of micro-sized container by making the hollow cavity inside. Meanwhile the study of functionalization of foldecture is expanding, it is ture that comprehending the self-assembly process and its resultant 3D shapes was harldy completed. For this reason, the structure determination of foldecture’s molecular packing structure was essential. At this point, powder X-ray diffraction technique was selected, due to the foldecture’s dimensions and kinetical experimental conditions. PXRD analysis, using synchrotron radiation, was adequate to determine the packing structure with well-organized bond and angle restraints. Further, it was able to designate absolute orientation of consisting foldamers, based on expected preferred orientation approximation. Application of PXRD analysis to foldecture was not only helpful to understand its shape and properties of the newly formed foldecture, but expected to play a huge role in designing the original foldecture in future.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-565**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

축산물분야(버터 중 산화방지제) 표준시료 개발 프로세스 연구

이기원

한국화학융합시험연구원 표준적합성운영팀

‘검사능력관리’란 ‘숙련도시험’을 의미하며 시험기관 간 비교를 통하여 시험 수행도를 판정하는 것으로 시험소의 능력을 평가하고 다른 시험소와의 편차식별, 발견된 문제의 원인파악 및 시정조치를 통해 시험소의 수행능력을 향상시키고자 실시된다. 국제적 기준(ISO Guide 34 및 KS Q ISO/IEC 17043)에 부합하며 균질성 및 안정성이 확보된 표준시료개발 및 검사능력관리를 통한 축산물시험검사기관 시험결과의 신뢰성 점검은 품질보증체계 확립에 중요한 역할을 하고 있다. 시험검사기관은 식품위생법 제 24 조 제 1 항에 의거, ‘...제 16 조 제 2 항의 규정에 의한 수입식품 등의 검사와 제 17 조 제 1 항의 규정에 의하여 수거한 식품 등의 검사에 관한 사무를 행하게 하기 위하여 그에 필요한 시설을 갖춘 기관...’을 뜻한다. 검사능력관리 평가분야는 이화학검사, 미생물검사, 유전자재조합식품검사로 분류된다. 해당 연구는 이 중 이화학검사분야 중 식품첨가물에 대한 검사능력관리에 대한 표준시료 개발 및 검사능력관리에 대해 다루고 있다. 축산물 이화학분야 중 산화방지제 분석용 표준시료 개발을 진행하였다. 산화방지제는 자신이 먼저 산화되고 이어서 지방이 산화(산패)되므로 유지의 산화속도가 억제되면서 산패가 발생되기까지의 시간(유도기간 : induction period)도 연장된다. 따라서 항산화제란 유도기간을 연장시켜 주는 물질이라고 말할 수 있으며, 산화방지제의 허용기준은 유지 및 버터에 있어서 다이뷰틸하이드록시톨루엔(BHT) · 삼차뷰틸하이드로퀴논(TBHQ) · 뷰틸하이드록시아니솔(BHA) 등의 첨가를 하는 경우에는 사용량을 200 mg/kg 이하 규정하고 있다. 버터 중 산화방지제 분석용 표준시료의 제조 프로세스를 연구/확립하고, 표준시료의 확보에 있어서 가장 중요한 균질성/안정성을 검증하여 숙련도평가용 시료로 적합한 표준시료를 개발하였다. 이번 검사능력관리 운영으로 제작된 시료는 시험검사기관 지정 및 평가를 위한 표준시료로 활용 되었으며, 시험검사기관의 분석에 대한 정확성 향상 및

국제적 동등성 확보를 위한 운영시스템을 확보하는 데 기여했다. 또한, 시험검사기관 검사능력관리를 위한 표준시료 개발 사업을 통해 국제기준(KS Q ISO/IEC 17043, 적합성평가·숙련도시험 일반 요구사항)에서 요구하는 균질성이 확보된 표준시료 개발 및 공급으로 국제적 수준의 검사능력관리에 대한 기반을 마련했다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-566**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Ru Substituted α-$Mn_{1-x}Ru_xO_2$ Nanowire as an Efficient Bifunctional Electrocatalyst for Oxygen Evolution and Reduction Reactions

강보현 JINXIAOYAN 오승미 황성주*

이화여자대학교 화학·나노과학과

Highly efficient bifunctional electrocatalysts of Ru-substituted α-$Mn_{1-x}Ru_xO_2$ nanowires are synthesized by one-pot hydrothermal method. The Ru substitution for α-MnO_2 nanowire leads to a decrease of aspect ratio with an increase of surface area. Also, electrical conductivity and charge transfer kinetics improve upon the Ru substitution. Substitution of Ru^{4+} ion in the octahedra Mn site of α-MnO_2 resulted in high oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) activities, which are superior to and/or compatible with those of commercial Ir/C and Pt/C. The incorporation of more covalent Ru-O bond gives rise to the weakening of neighboring Mn-O bond via the bond competition, the weaker Mn-O bond causes stabilization of unstable Jahn-Teller distorted Mn^{3+} ions that play an important role in O_2 species transition. The present work clearly demonstrates that the Ru substitution for α-MnO_2 nanowire is highly effective in improving the bifunctional electrocatalytic activities of ORR and OER.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-567**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Using Core/Shell($Fe_3O_4@SiO_2$) Nanoparticles Immobilized with CD(β-Cyclodextrin) to Detect and Separation of Dyes

홍상은 장경주 윤국로*

한남대학교 화학과

Cyclodextrins were formation of host-guest complexes with hydrophobic molecules and these molecules have found of applications in a detect and separation system. Preperation of uniformly sized silica-coated magnetic nanoparticles were synthesized in a simple one-pot process using reverse micelles as nanoreactors. Surface modified of core/shell($Fe_3O_4@SiO_2$) nanoparticles were prepared from the reaction core/shell nanoparticles immobilized by monochlorotriazinyl-β-cyclodextrin (MCT-β-CD).We reported core/shell($Fe_3O_4@SiO_2$) nanoparticles immobilized with CD(β-Cyclodextrin) for detect and separation of methylene blue dye as a model compound. The resulting hybrid nanoparticles was confirmed by FE-SEM(Field-emission Scanning Electron Microscope), FE-TEM(Field-Emission Transmission Electron Microscope), Energy Dispersive X-ray Spectroscopy, FT-IR(Fourier Transform Infrared Spectroscopy), DLS(Dynamic Light Scattering), TGA(Thermogracimetric Analysis), ^{1}H-NMR(1H Nuclear Magnetic Resonance) and ESI-MS(Elextrospray Ionization-Mass Spectrometry).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-568**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

전기방사법을 이용한 해양복합고분자 (Chitosan/Fucoidan/Glycosaminoglycans) 나노섬유 제작 및 물성평가

오태석 장경주 홍상은 윤국로*

한남대학교 화학과

나노섬유는 높은 비표면적, 공극률 및 구조와 크기 조절이 용이해 조직/재생 의공학적, 고성능 필터 소재, 바이오센서, 화장품 소재 등의 응용 분야에서 연구되고 있다. 키토산(Chitosan)은 생체 친화적, 생분해성 등의 생물학적 특성이 우수한 천연고분자이다. 후코이단(Fucoidan)과 글리코사미노글리칸(Glycosaminoglycans)은 다양한 생리활성을 나타내는 황산기를 가지고 있다. 본 연구는 전기방사(Electrospinning)를 이용하여 해양 복합 고분자(Gelatin/ Chitosan/ Fuciudan/ Glycosaminoglycans)을 함유하는 나노섬유를 제조 하였다. 제조된 복합나노섬유의 물성을 평가하기 위해 광학현미경(Optical microscopy), 주사전자현미경(Scanning Electron Microscopy), 적외선분광기(Fourier Transform Infrared Spectroscopy), 열중량분석(Thermogravimetric Analysis), 인장강도(Tensile stress-strain)를 확인하였다

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-569**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

전기방사법(Two-nozzle method)을 이용한 Agarose/PCL-Fucoidan 복합섬유의 제조 및 특성

김재경 홍상은 장경주 윤국로*

한남대학교 화학과

아가로스(Agarose)와 PCL-후코이단(Fucoidan)을 전기방사(two-nozzle method)하여 복합섬유를 제조하였다. 복합섬유에 사용된 아가로스(agarose)는 홍조류로부터 추출된 다당류로 독성이 없으며 우수한 생체적합성과 수분함유도로 화상치료제로서 의약분야에도 많이 연구 되고 있다. 후코이단(fucoidan)은 갈조류로부터 추출된 다당류로 생체조직을 보호하고 상처를 치유하며 염증을 예방하는 효과가 있다. 본 연구에서 제조된 복합섬유는 주사전자현미경(Scanning Electron Microscope)을 통해 각각 서로 다른 굵기를 보이는 아가로스(Agarose)/PCL-후코이단(Fucoidan) 나노섬유를 확인하였으며 아가로스(Agarose) 함유량에 따라 수분흡수율이 크게 증가함을 확인하였다. 복합섬유는 아가로스(Agarose) 단일 섬유보다 물성이 증가함을 확인하였다. 제조된 복합섬유의 특성은 광학현미경(Optical Microscope), 주사전자현미경(Scanning Electron Microscope), 인장력(Tensile Strength), 접촉각(Contact Angle), FT-IR, 열 중량 분석(Thermogravimetric analysis), 수분흡수율(Water uptake)을 통해 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-570**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

해양유래물질(키토산/ 후코이단/ 글리코사미노글리칸)을 함유한 다공성 하이드로겔의 제작 및 물성평가

김용운 장경주 홍상은 윤국로[*]

한남대학교 화학과

하이드로겔은 물에 팽윤할 수 있는 망상 구조로서 수용액 내에서 다량의 물을 내부에 함유할 수 있는 고분자 이다. 하이드로겔은 마스크팩, 콘택트렌즈, 상처치료제등 다양한 분야에서 연구되고 있다. 해양천연물을 함유한 하이드로겔의 경우 피부에 대한 자극, 가려움 등의 부작용이 적을 뿐만 아니라 피부의 효소반응에 의해 직접적으로 피부에 유효한 효과를 줄 수 있다는 장점이 있다. 본 연구에서는 해양유래물질인 키토산, 후코이단, 글리코사미노글리칸을 이용하였다. 키토산은 미세먼지와 피지를 흡착하는 특성이 있고, 후코이단은 효과적인 보습효과와 미백효과를 가지고 있다. 글리코사미노글리칸은 항산화, 항염효과를 나타낸다. 해양유래물질을 함유한 하이드로겔은 키토산 용액과 후코이단/글리코사미노글리칸 용액, 젤라틴 용액을 60 ℃에서 5 분간 교반 후 4℃에서 24 시간 동안 경화하였다. 다공성 하이드로겔을 제작하기 위해 24 시간 동안 동결건조를 진행하였다. 제작한 다공성 하이드로겔은 주사전자현미경(SEM), 접촉각(contct angle), 팽윤도(Degree of swelling), 감쇠전반사도(ATR), 열중량분석(TGA), 인장강도(Tensile strength)를 확인하였다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-571**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fabrication of InGaN-based nanorod light-emitting diodes as planar surface light sources

어윤재 유강열[1] 이영기 김웅[2] 도영락[3,*]

국민대학교 화학과 [1]고려대학교 신소재공학과 [2]고려대학교 신소재공학부 [3]국민대학교 생명나노화학과

In this study, we fabricated the millions of 1-dimensional (1D) nanorod light-emitting diodes (LEDs) using polystyrene (PS) nanosphere lithography, etching and cutting process of InGaN/GaN LED structure epi-wafer. Additionally, we produced a surface LED device with large area (0.7 cm x 0.6 cm) using individually separated 1D nanorod LEDs by electric field-assisted assembly method on pre-patterned electrodes. The assembled green InGaN-based nanorod LED device exhibits maximum luminance of ~2,130 cd/m^2, current efficiency of ~1.65 cd/A, and power efficiency of ~0.95 lm/W after post-treatment. Despite of low electrical performance, the device could be improved by interconnection between nanorod LEDs and electrodes (ohmic contact) and high purity nanorod LEDs. As a result, the assembled nanorod LEDs can be used as a planar surface emitting applications such as displays and lightings.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-572**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

트립신이 고정화된 실리카 코팅 자성 나노입자의 제조 및 특성

박세웅 홍상은 윤국로*

한남대학교 화학과

균일하고 안정한 코어/쉘 나노입자(Fe3O4@SiO2)의 합성과 나노입자 표면에 트립신을 고정하였다. 이러한 실리카 코팅 자성 나노입자는 표면적 대 체적비가 높아 다량의 트립신을 고정하는데 용이하다. 본 연구에서는 코어/쉘 나노입자(Fe3O4@SiO2)에 트립신을 고정하기 위해 코어/쉘 나노입자(Fe3O4@SiO2) 표면에 링커로서 글루타알데하이드를 도입하여 트립신을 고정화하였다. 링커의 역할로는 고정화된 트립신의 안정성과 활성을 향상시킬 수 있다. 나노입자의 표면에 고정된 효소는 그 활성을 더 높일 수 있고 분리나 회수을 자성을 이용하여 진행하여 생물 의학 분야에 적용 시킬 수 있다. 얻어진 코어-쉘 나노 입자는 투과전자현미경(TEM), 주사전자현미경(SEM), 동적광산란법(DLS), X-선 회절(XRD), 적외선분광기(FT-IR), 에너지 분산 형 분광 분석법(EDS)를 이용하여 특성을 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-573**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

Optimization of CO_2 Adsorptivity of Layered Double Oxide via co-hybridization with Graphene and Layered Metal Oxide Nanosheets

<u>Haslinda binti Mohd Sidek</u> 조윤경[1] 황성주[2,*]

이화여자대학교 화학·나노과학 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학·나노과학과

A novel approach is developed to explore an efficient CO_2 adsorbent via the incorporation of layered double hydroxide (LDH) in the hybrid matrix of reduced graphene oxide (rG-O) and layered titanate nanosheets, and the following calcination at elevated temperature. The stabilization of layered double oxide (LDO, $MgO/MgAl_2O_4$) in the hybrid matrix of rG-O and layered titanate nanosheets is accomplished by an electrostatically-derived self-assembly between cationic Mg-Al-LDH nanosheet and anionic graphene oxide (G-O)/layered titanate nanosheet followed by heat-treatment. The co-hybridization with titanate and rG-O nanosheets caused a remarkable surface expansion of LDO ($MgO/MgAl_2O_4$), indicating the formation of open network with large pores. Of prime importance is that the incorporation of very small amount of layered titanate (0.3wt %) induces a significant expansion of surface area of $MgO/MgAl_2O_4$-rG-O nanocomposite from 178 to 330 m^2 g^{-1}. The resulting $MgO/MgAl_2O_4$-rG-O-layered titanate nanocomposite exhibits quite promising CO_2 adsorption capability of 1.71 mmol g^{-1} at 273 K, which is much higher than those of $MgO/MgAl_2O_4$ (0.79 mmol g^{-1}) and $MgO/MgAl_2O_4$-rG-O nanocomposite (1.19 mmol g^{-1}), highlighting the prominent effect of titanate addition on the gas adsorption functionality of LDO-graphene nanocomposite. The present study clearly demonstrates the effectiveness of the hybridization rG-O and layered metal oxide nanosheets for enhancing the gas adsorption capacity of LDO resulted from the calcination of LDH.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-574**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mode Coupling of Surface Plasmon Polaritons on Metallic Nanostructures

김화평 이민형*

경희대학교 응용화학과

Ordered hollow nanodomes carved in Au film were fabricated using anodic aluminum oxide as a template for Au deposition. The hollow Au nanodomes with retain the well-ordered structures of AAO mold with square or hexagonal arrays. The nanodomic Au film is interesting plasmonic crystal with tunable plasmonic resonances depending on the amount of contact between Au film and glass substrate. Also, the plasmonic energy gaps are observed due to the mode coupling of distinct SPPs of strong air-Au modes and weak Au-glass modes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-575**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Laser Induced Patterning of Metallic Cobalt/Reduced Graphene Oxide Hybrids and its Energy Storage Applications

이상화 이민형*

경희대학교 응용화학과

With tremendous usage of hand-held electronic devices in these days, energy storage devices with higher power and capacity are desired. Electrochemical capacitor or supercapacitor has been attracted by high volumetric energy density, power density and fast charge-discharge rate. Graphene/metal hybrids often studied as an advanced material for energy storage devices because those can increase chemical and electrical interaction with advantage of graphene which possesses high surface area and electrical conductance.. In this work, reduced graphene oxides/ cobalt nanoparticle composite has been selectively grown by laser induced photothermal reactions on graphene oxide film. This composites exhibited an enhanced performance in micro-supercapacitor test.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-576**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Selective Annealing and Multi-morphology Patterning of Block Copolymer via Photothermal Annealing

김재겸 이민형*

경희대학교 응용화학과

Block copolymer is copolymer consist of two or more different types of polymer making single string. Block copolymer self-assembly is one way of bottom-up patterning method which can efficiently produce sub-10 nanometer size ordered pattern. By regulating the experiment condition, we can easily tune morphology and size of the block copolymer pattern. To self-assemble block copolymer, many different approaches have been developed. In many different methods of annealing block copolymer, thermal annealing and solvent annealing is the most widely used methods because of efficient methods and time. In this project, besides two methods mentioned above, we approached with photothermal annealing to self-assemble block copolymer in selective area with tunable morphologies. Photothermal annealing could be an efficient method to self-assemble block copolymer from the time spent view and processing view.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-577**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Crystal Structure of the New One-dimensional Palladium Thiophosphate, $KPdPS_4$•KI

윤우진 윤호섭[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

The new palladium thiophosphate, $KPdPS_4$•KI, has been synthesized through alkali metal halide flux methods and structurally characterized by single crystal X-ray diffraction techniques. The title compound crystallizes in the space group Pnma. Each palladium atom is surrounded by four sulphur atoms in the square planar fashion and phosphorus atoms are coordinated by four sulphur atoms in a tetrahedral geometry. The polyhedra are combined to form the one-dimensional infinite anionic chains, ${}_{\infty}^{1}[PdPS_4^-]$. Alkali metal and halide ions (K^+ and I^-) reside among the chains to complete the three-dimensional structures. The classical charge valence can be described as $[K^+][Pd^{2+}][P^{5+}][S^{2-}]4•[K^+][I^-]$.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-578**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A new member of the $A_2MB_3Q_8$ (M=divalent Transition Metals, A=Alkali Metals, B=Si, Ge, Q=Chalcogens) Family: Synthesis and structure of the mixed-metallic $Rb_{2-2x}Mn_{1-x}Ge_{3+x}Se_8$

이준구 윤호섭[1,*]

아주대학교 에너지시스템학부 응용화학과 [1]아주대학교 화학과

In our group, a number of new phases in the $A_2MB_3Q_8$ family (M=transition metals, A=alkali metals, B=Si, Ge, Q=chalcogens) have been synthesized through alkali metal halide flux methods and their structures have been determined by single crystal X-ray diffraction techniques. These compounds have various structural type from 1-dimensional to 2-dimensional. In addition, the 2-dimensional layers can be divided into two structural types according to the preferred metal coordination. In this presentation, we will present synthesis and structure of a new mixed-metallic member of this family, Comparison among the different structures will be given as the relationship between stoichiometries of transition metals and occupancy of alkali metals. The charge valance of the compound can be described as $[A^+]_{2-2x}$ $[M^{2+}]_{1-x}[B^{4+}]_{3+x}[Q^{2-}]_8$, which is compatible .

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-579**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Porous Polymer for Precious Metal Capture

홍영란 YAVUZCAFERTAYYAR[1,*]

KAIST EEWS [1]KAIST EEWS 대학원

Precious metals indicate the coinage group of silver and gold and the platinum group of ruthenium, rhodium, palladium, osmium, iridium, and platinum. These metals are highly valuable and used in diverse industries due to their superior properties such as high stability, electrical conductivity, ductility, luster, and catalytic properties. Because precious metals are limited resources, the mining of these metals should be broadened from natural ores to secondary sources such as industrial wastewater or natural water. The current technologies for precious metal recovery from the secondary sources are pyrometallurgy, hydrometallurgy, and biometallurgy. However, these methods are limitedly applied in the electronic wastes and require high energy costs and hazardous organic solvents. The research on solid adsorbents for recovering precious metals from water sources is very deficient. Therefore, the solid adsorbents for selectively capturing and recovering precious metals should be developed. In this study, the adsorbent, COP180, was synthesized. The structure of the prepared polymer was characterized by several analytical methods such as Fourier transform infrared spectroscopy, elemental analysis, Brunauer, Emmett and Teller analysis, and high resolution mass spectrometry. The metal selectivity test results show that the polymer selectively captures precious metals among almost all metals in the periodic table with over 90 % efficiency.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-580**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mechanism of PEDOT:PSS Conductivity Enhancement by Ionic Liquids: DFT Study

박성진 장윤희[1,*]

GIST 신소재공학부 [1]DGIST 에너지시스템공학

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate), so-called PEDOT:PSS, is a water-processible transparent conducting polymer. It could replace the conventional transparent electrode ITO, but the conductivity is still not satisfactory. The low conductivity of the PEDOT:PSS film is attributed to the formation of core-shell nanoparticles, in which the hydrophilic (but insulating) PSS outer layers encapsulate the conducting (but hydrophobic) p-doped PEDOT cores. Recently a significant conductivity enhancement has been achieved by adding ionic liquid (IL) in the PEDOT:PSS solution. It is believed that ion exchanges between PEDOT, PSS, and IL components help PEDOT decoupled from PSS and to grow into large-scale conducting domains although the exact mechanism is still under debate. Hence we carry out density functional theory (DFT) calculations to evaluate the free energy of ion exchange between PEDOT:PSS oligomer and a series of IL pairs. The calculations indeed show that the most efficient IL additives among the series (which has been observed to induce 5000 times of conductivity enhancement) are the least tightly bound IL pairs with the lowest binding energies which result in the most negative free energies of ion exchange (in other words, the most spontaneous ion exchange with PEDOT:PSS). Based on such design rule, new IL pairs with even lower binding energies are designed and suggested as promising IL additives. In addition, since the residual IL components remaining in PEDOT domains could cause a doping effect to further enhance the conductivity, DFT-based non-equilibrium Green's function calculations are performed to evaluate the tunneling currents of a single thread of PEDOT oligomer decorated by the same series of IL components after the ion exchange reaction. We indeed find that the high-performance IL additive induce not only a spontaneous ion exchange with PEDOT:PSS to improve the PEDOT morphology but also a partial oxidization (in other words, p-doping) of PEDOT to enhance its intrinsic conductivity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-581**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Simple preparation method and characterization of sodium carboxymethyl cellulose/polyethyleneimine composites

손영래 박수진*

인하대학교 화학과

Sodium carboxymethyl cellulose/polyethyleneimine (CMC/PEI) composites were fabricated as a function of PEI contents by a simple solution mixing and casting method. The anionic CMC and cationic PEI were combined by ionic interaction. The characterization and mechanical behaviors of CMC/PEI composites were analyzed using X-ray diffraction (XRD), scanning electron microscope (SEM) and universal testing machine (UTM). Concretely, the structural properties and morphologies of CMC/PEI composites were investigated by using XRD and SEM, respectively. The mechanical behaviors of CMC/PEI composites were analyzed by UTM. It was found that tensile strength and Young's modulus of CMC/PEI composites were slightly decreased, but failure strain was increased.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-582**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Clear-cut observation of clearance of injected cargoes from lymphatic system of small living mice by using high-quality NIR-to-NIR upconversion luminescence imaging

남상환 김종우[1] 서영덕[1,*]

한국화학연구원 나노바이오융합연구센터 [1]한국화학연구원 나노라만융합연구센터

Lanthanide-doped upconverting nanoparticles (UCNPs) with unique optical advantages like a photo- and chemical-stabilities are suitable for research field of in vivo optical imaging. UCNPs do not make an issue of noise caused by autofluorescence background, providing a great signal-to-noise ratio. Especially, Tm^{3+}-doped UCNPs are often utilized for long-term non-invasive in vivo optical imaging and tracking. Herein, to understand excretion pathways and clearance of injected cargoes from lymphatic system of small living mice, transport and retention of the UCNPs in the lymphatic system were evaluated with high-quality NIR-to-NIR upconversion luminescence (UCL) imaging. We obtained their kinetic luminescence profiles for the injection site and sentinel lymph node (SLN) and observed luminescence signals for one month, and we also examined UCL images in SLN tissues, organs, and faeces at each time point. We understand that the injected UCNPs in a footpad of a small mouse are transported rapidly from the lymphatic system to the blood system and then eventually result in an efficient excretion by the hepatobiliary route.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-583**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis of narrow-band emitting red K_2SiF_6:Mn^{4+} phosphor for realization of high color quality white LEDs

강희준 오지혜 도영락*

국민대학교 생명나노화학과

In this study, we successfully synthesized a narrow-band red-emitting K_2SiF_6:Mn^{4+} phosphor using a facile etching method in order to realize high color quality warm-white LEDs with high luminous efficacy. The narrow-band red-emitting K_2SiF_6:Mn^{4+} phosphor-converted LED (pc-LED) with a long-wavelength pass dichrioc filter (LPDF) shows pure deep red color and thermally stable. We compared optical properties such as a luminous efficacy (LE), a color rendering index (CRI) and newly developed TM-30-2015 (R_f and R_g) of four-package white LEDs, which are composed of an InGaN blue LED and LPDF-capped green/amber/red pc-LEDs by changing the red phosphors (a narrow-band K_2SiF_6:Mn^{4+} phosphor and five kinds of wide-band (Ca,Sr)$SiAlN_3$:Eu^{3+} phosphors) at various correlated color temperature (CCT) from 2700 K to 6500 K. The four-package white LED including a K_2SiF_6:Mn^{4+} LPDF-capped pc-LED shows high LE (107 ~109 lm/W) and great color qualities (CRI = 92~94, R_f = 79~81.5, R_g = 101.4~102.5) at the warm-white CCT ranges from 2700 K to 3500 K. The K_2SiF_6:Mn^{4+} phosphor is a good candidate for realization of highly efficient and excellent color quality warm-white LEDs.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-584**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation on hexagonal disk form of $NaLuF_4$:Yb,Er,Gd upconversion material

B.T.Huy 이용일[1,*]

창원대학교 화학과 [1]창원대학교 화학과

The uniform hexagonal disk-shaped of Gd^{3+},Yb^{3+},Er^{3+}-codoped $NaLuF_4$ upconversion material has been successfully prepared using hydrothermal route. The prepared samples possess good fluorescent emission under laser excitation at a wavelength of 980 nm. The effect of synthetic conditions, such as the precursor concentration, pH values, and temperature on the shape was detailed. The possible formation and upconversion mechanisms were proposed. This study is expected to provide information for controlled synthesis of other upconversion materials.

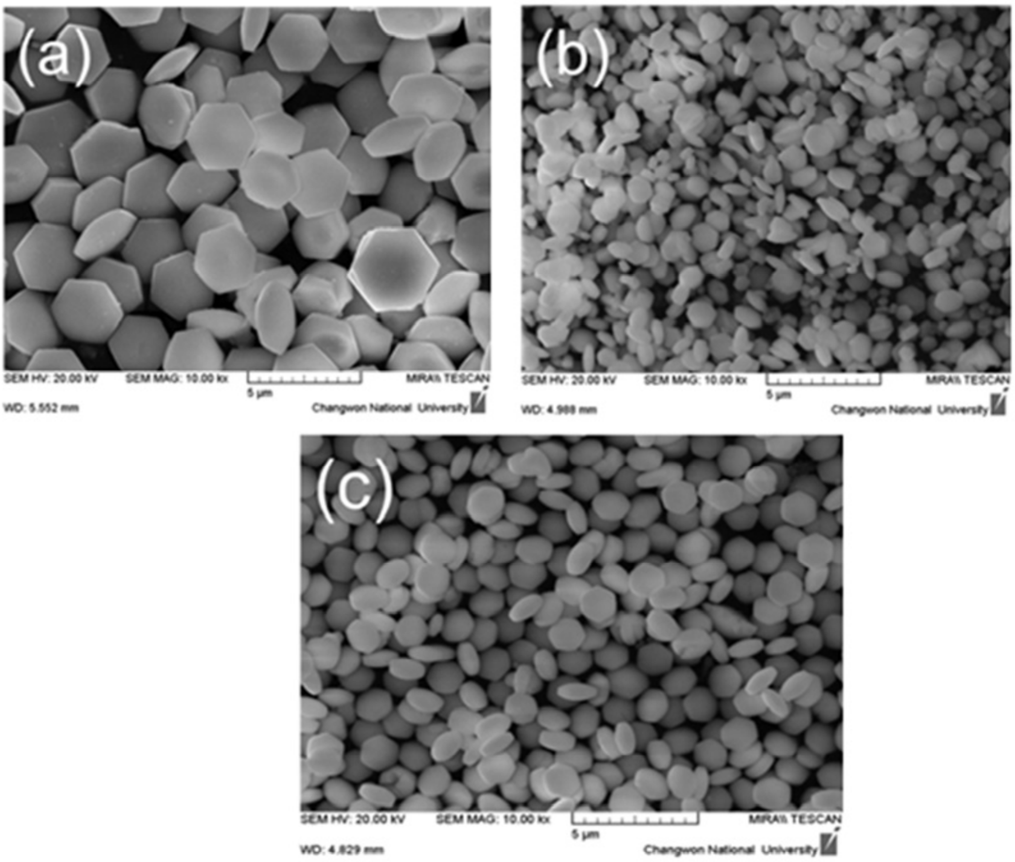


Figure: Effect of $RE(NO_3)_3$ concentration at 6 mmol NaF: 150 mg (a), 300 mg (b), and 400 mg (c).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-585**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enhanced CO2 Uptake by Pentaethylenehexamine Impregnation on UiO-66-NH2

송영동 YAVUZCAFERTAYYAR[1,*]

KAIST EEWS 대학원 [1]KAIST EEWS 대학원

The concentration of carbon dioxide in the atmosphere has been increasing, which has been causing serious problems such as global warming and ocean acidification. In order to control CO2 emissions, the effectiveness of many solid adsorbents are studied. Metal organic frameworks (MOFs) are among the promising solid CO2 adsorbents. Of all the MOFs, UiO-66-NH2, amine functionalized UiO-66, is an attractive candidate because it has high thermal and chemical stability and inherent primary amine. In addition, many kinds of amine molecules can be impregnated to increase CO2 uptake due to high affinity of nitrogen in amine functional group to CO2. Here, we introduce the first pentaethylenehexamine impregnation into UiO-66-NH2 and in various ratios for optimization. Our results show enhanced CO2 uptake at low pressure region, which is ideal for post-combustion CO2 adsorption processes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-586**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enhanced adsorption and desorption kinetics of CO2 of Li4SiO4 via lithium ion channelling effect using TiO2 nanotubes

이주성 **YAVUZCAFERTAYYAR**[1,*]

KAIST EEWS 대학원 [1]KAIST EEWS 대학원

Lithium silicate (Li¬4SiO4) through its chemisorption reaction, has attracted extensive scientific research from its large CO¬2 adsorption capacity at high temperature with low cost to synthesize. However, the conventional nonporous Li4SiO4 shows very poor CO2 adsorption kinetics. Thus, Li4SiO4-TiO2 complex was synthesized where LiOH and fumed silica would form around TiO¬2 nanotube. With TiO2 nanotube in LI¬4SiO4 structure, lithium ions were able to channel through the bulky structure and enhance not only the kinetics but the total adsorption capacity to near theoretical value. Through absorption and desorption studies, Li4SiO¬4-TiO2 complex has shown significantly improved uptake capacity and kinetics. Furthermore, Cyclic studies were examined at 700oC and has shown strong stability after 10 cycles. As there are various ways of forming TiO2 nanotube, their stability will vary in high temperature and must be applied in Li4SiO4 for optimal stability of overall structure.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-587**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of fluorescent silica-coated iron oxide nanoparticles for dual modal in vivo MR and fluorescence tumor diagnosis

이채동 유동건 박원철*

서울대학교 융합과학기술대학원 융합과학부

In this research, we prepared fluorescent silica-coated iron oxide nanocrystals for dual fluorescence and magnetic resonance imaging. The as-prepared core/shell nanoparticles were intended to improve the diagnostic accuracy and broaden the scope of the diagnosis. In the synthesis, the as-prepared iron oxide nanocrystals were coated with RITC (Rhodamine B isothiocyanate)-doped silica shell via reverse micelle method. Then the core/shell nanoparticles were analyzed to confirm the shape, size distribution and fluorescence by transmission electron microscopy (TEM), dynamic laser scattering (DLS) and photoluminescence (PL) spectroscopy each. By WST-1 assay, we confirmed that the as-prepared nanostructures are not toxic in cell levels. Finally, through in vivo MR and fluorescent imaging, we verified its possibility as bimodal imaging contrast agents for cancer diagnosis.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-588**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Evaluation of the color quality properties of InP/ZnS quantum dots based white LEDs using CRI and TM-30-2015

김소희 오지혜[1] 김찬식 도영락[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

In this study, we synthesis green, amber, and red emitting InP/ZnS quantum dots (QD) and realization of InP/ZnS QD based white LEDs with various correlated color temperature (CCT) of 6,500 K ~ 2,700 K. Also, we measure the optical properties such as luminous efficacy (LE), color rendering index (CRI, R_a) and TM-30-2015 (R_f and R_g) of the InP/ZnS QD based white LEDs. Many researchers in the field of white LEDs usually evaluate the white color quality using only CRI. However, the CRI are limited in their inability to guarantee good saturated red, green, and blue colors of illuminated objects under a warm white color. To overcome the CRIs problem, a two-measure system (TM-30-2015) was developed and adopted as Illuminating Engineering Society of North America (IES) including the color fidelity score (CFS, R_f) and the color gamut score (CGS, R_g). Therefore, we introduce TM-30-2015 and measured InP/ZnS QD based white LEDs using not only CRI but also TM-30-2015.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-589**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Up-conversion luminescence properties in Lanthanide nanoparticles by cross relaxation mechanism

정종원 GerelkhuuZayakhuu 이용일[*]

창원대학교 화학과

Lanthanide doped upconversion nanoparticles (UCNPs) have been widely applied in a variety of areas as optical devices, sensing, and therapeutics. Their advantages include near infrared (NIR) excitation that low toxicity, weak autofluorescence, high chemical stability, and low photo bleaching. The UCNPs are a process that generates higher energy emission from the low energy of incident light. Many trivalent rare earth ions including Er^{3}+, Tm^{3}+ and Ho^{3}+ are doped in emission and absorption centers in these materials. Recently, the UC phosphors have attracted much attention due to their potential applications in various fields, such as solid-state lasers, solar energy converter, and bio-sensors. Among these applications, considerable attention is devoted for bio-sensor applications. UC phosphors can use near-infrared (NIR) instead of conventional ultraviolet (UV) as an excitation source, which has many advantage such as no reaction with tissues and high quantum efficiency on nanoparticles. The $NaYF_4$ host lattice is well known material as one of the most efficiency host lattices. In this study, we synthesized the Yb^{3}+, Er^{3}+ and 4f-ions co-doped $NaYF_4$ with nanoparticles materials. The UC properties of Yb^{3}+, Er^{3}+ and 4f-ions co-doped $NaYF_4$ phosphors were investigated by varying the 4-f ions energy transition mechanism. We confirmed that the UC luminescence efficiency was enhanced by cross relaxation from various 4f-ions. The emission spectra of all phosphors reveal mainly two colors, correspond to green and red transition of Er^{3}+ and 4-f ions. The 4-f ions co-doped $NaYF_4$ phosphors have pure red or green emission spectra. We examined the UC luminescence mechanism using a decay time, pump power dependence and energy level diagram by cross relaxation mechanism.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-590**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Preparation of uniform ferrite nanoparticle by metal2+-acetate precursor

정의석 **YAVUZCAFERTAYYAR**[1,*]

KAIST EEWS [1]KAIST EEWS 대학원

Recently, iron oxide nanoparticle and ferrite (Metal-Fe2O4) structure has been enormously developed not only its physical, chemical, magnetic property but also for many technological applications: drug delivery, mechanical fluid, magnetic storage media, contrast agents in magnetic resonance imaging (MRI), and magnetic fluorescence dye. Furthermore, the control of the uniform particle size is very important parameter because the physical and chemical properties of the MR fluid depend on particle structure, crystallinity and dispersity. In this work, to improve applications and magnetic property of MR fluid, the ferrite (MeFe2O4) nanoparticles are synthesized using iron hydroxide and Co, Cu, Ni metal-acetate precursor in 1-octadecene and oleic acid. Particle size and structural properties were determined and compared using X-ray diffraction (XRD), Transmission Electron Microscopy (TEM).Keywords: Iron oxide nanoparticle, Cobalt, Copper, Nickel, ferrite.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-591**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Printing-based thermoelectric sensors for digital microfluidic chip on paper

채희도 정해나[1] Veasna Soum[1] 권오선[1,*] 신관우[2,*]

서강대학교 화학과 대학원 [1]서강대학교 화학과 [2]서강대학교 화학과 및 바이오융합과정

As microfluidic chip is designed 15 years ago, hundreds of researches proposed applications of microfluidic chips such as polymerase chain reaction(PCR) and synthesis of gold nanoparticle. But the heating up of solution is still a challenging process and needs complicated steps to make a heater on chip. In this research, we made digital microfluidic chip on photopaper with thermoelectric sensor to monitor temperature of heater and samples. Microfluidic chip is printed with MWCNT/Screen ink, Ag nanoparticle by Screen printing and inkjet printing for each. To make thermoelectric sensor, PEDOT:PSS electrode is fabricated by screen printing. Screen printing provides thick electrode layers for both CNT and PEDOT:PSS. These electrode can maximize Seebeck effect and show enough conductive to move droplet by electrowetting on dielectric layer(EWOD). Dielectric layer is fabricated with SU-8 photoresist, which is commonly used for the fabrication of microfluidic devices. Additional hydrophobic layers like Teflon and silicon oil are spin-coated if needed. These microfluidic devices can move droplet on the paper while sensing temperature simultaneously. These chips can be used for point of care(POC) devices for being easily fabricated and deposable.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-592**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Controlled synthesis of highly multi-branched Ptbased alloy nanocrystals with high catalyticperformance

김예나 한상우*

KAIST 화학과

Alloy nanocrystals (NCs) consisting of Pt and a 3d transition metal (M) have been of tremendous interest due to their prominent catalytic performance. To precisely compare the inherent catalytic function between PtM NCs with different M elements and thus to find an optimal combination, the availability of a synthesis method that provides exclusive control over the M element is highly desirable. In the present work, we developed a general solvothermal synthesis method for the preparation of highly multi-branched PtM (M = Co, Ni, and Fe) alloy NCs with similar branch dimensions, compositional ratios between Pt and M, and surface chemical environments, irrespective of the identity of M. Using the methanol oxidation reaction (MOR) as a model catalysis reaction, we found a correlation between the catalytic capabilities of the PtM NCs and the kind of the secondary metal. The MOR activity of the PtM NCs outperformed that of a benchmark Pt/C catalyst, and it distinctly depended on the identity of M. The enhanced catalytic function of thePtM alloy NCs compared to Pt/C can be attributed to their unique structural characteristics and the decrease in the binding energy of intermediates due to the synergism between Pt and M. Among the different PtM alloy NCs, the PtCo NCs exhibited the highest catalytic activity, stability, and CO tolerance due to the effective modification of their surface electronic structure. The present strategy can expand our opportunities for the rational design of advanced NC catalysts with controlled morphological, compositional, and electronic structures.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-593**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

[발표취소] Multiscale Simulations of Charge Transport Properties in Organic Semiconductors: Effect of Morphology in P3HT(poly-3-hexylthiophene) and PCPDT-BT(poly-cyclopentadithiophene-benzothiadiazole) Photovoltaic Donor Materials

김영록 유택희[1] 장윤희[*]

DGIST 에너지시스템공학 [1]GIST 신소재공학부

발 표 취 소
본 논문은 발표취소된 논문입니다.

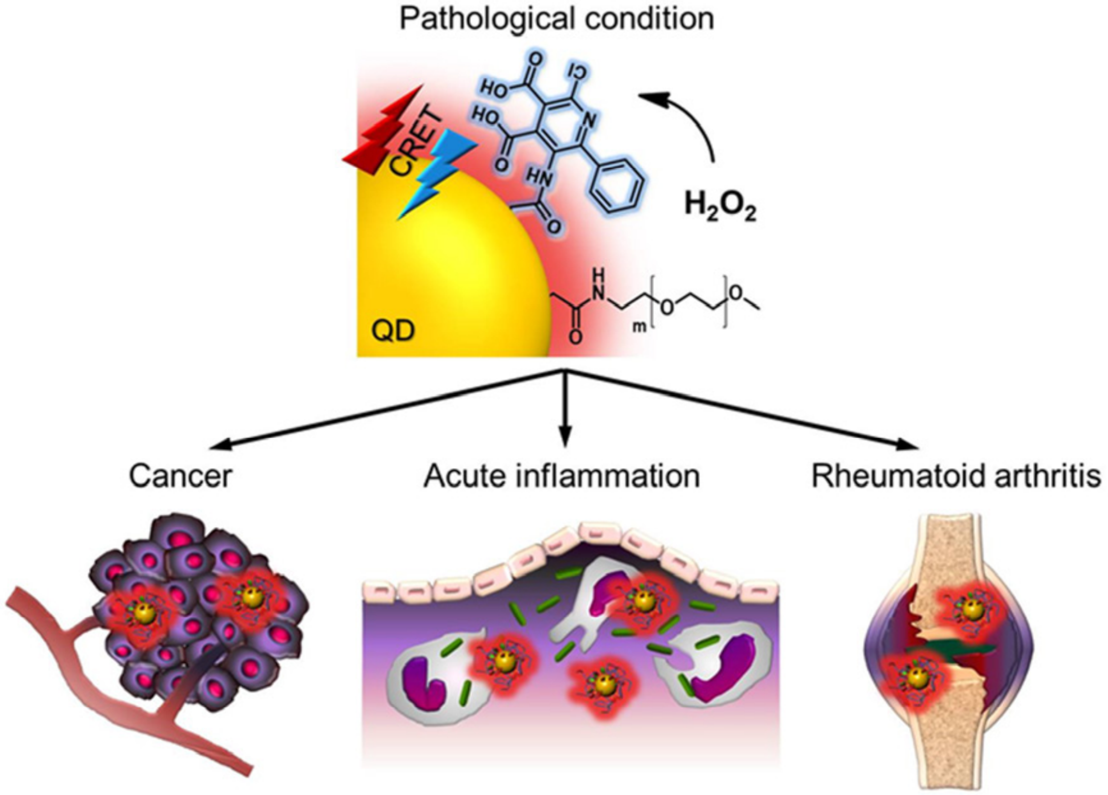
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-594**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Nanoconjugates Based on Quantum Dots and a Luminol Derivative: Implications for *in vivo* Imaging of Hydrogen Peroxide

이은숙 박재형[1,*] 서영덕[2,*]

성균관대학교 융합의과학과 [1]성균관대학교 화학공학부 [2]한국화학연구원 나노라만융합연구센터

Reaction oxygen species (ROS), produced by incomplete reduction of oxygen, play a role in functions ranging from cell homeostasis to cell death as signaling molecules. Overproduction of hydrogen peroxide, one of main ROS, is associated with the pathogenesis of inflammatory diseases such as cancer and rheumatoid arthritis. Herein, we have investigated potential of hybrid nanoparticles (HNPs), based on a luminol derivative (L012) and quantum dots (QDs), as the chemiluminescent agent for *in vivo* optical imaging of hydrogen peroxide without an external energy source. Since L012 produces energy by its specific reaction with reactive oxygen species, it was hypothesized that QDs in HNPs could emit near infrared (NIR) light via chemiluminescence resonance energy transfer (CRET). No significant NIR signals were observed from L012 or QD itself in the presence of hydrogen peroxide, whereas HNPs exhibited strong NIR intensity, inferring that L012 and QD served as the CRET donor and the acceptor, respectively. In addition, the NIR intensity generated from HNPs corresponded to the concentration of hydrogen peroxide. It should be noted that HNPs enabled *in vivo* imaging of hydrogen peroxide in animal models with prostate cancer, acute inflammation and rheumatoid arthritis. Overall, HNPs may have potential as a diagnostic agent for hydrogen peroxide-associated diseases.


Pathological condition
CRET
QD
HO
HO
Cl
N
HN
O
H
N
m
O
O
H_2O_2
Cancer
Acute inflammation
Rheumatoid arthritis

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-595**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A novel sensor for detecting thiols groups using upconversion fluorescence material

NGUYEN THI THU THUY B.T.Huy GerelkhuuZayakhuu 이용일*

창원대학교 화학과

The fluorescence sensor in a perfect combination of the upconversion fluorescence resonance energy transfer (FRET) process and derivative Rhodamine B (RBD) probe was designed to detect thiol groups sensitively and selectively. The derivative Rhodamine B bound on surface of UCP through electric statistics. Under optimized conditions, the sensor shows strong response and high linear Stern-Volmer characteristics through FRET between $NaLuGdF_4$:Yb,Er nanoparticles as the energy donor and RBD as the energy acceptor. Evidences suggests that, in the presence of thiols, the fluorescent energy transfer from UCP, which has emission at 550 nm, to RBD (absorbed at 550 nm), results to emit at 585 nm. The nanosensor is able to detect thiols in aqueous solution and distinguish different thiols. The sensing mechanis, characterizations of nanoparticles, and FRET process of prepared sensor towards thiols is discussed. The limit of detection for glutathione reaches to 0.5 μM. In future, the sensor will be estimated in real samples.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-596**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Highly selective optosensing for ibuprofen using CdTe quantum dots capped with natural amphiphilic alginate biopolymer

Salah Mahmoud Tawfik Ahmed **B.T.Huy** 이용일*

창원대학교 화학과

We present the facile synthesis of novel amphiphilic biopolymers derived from natural alginic acid as a capping agent for CdTe quantum dots (QDs) to overcome the main problems of traditional thiol instability and hydrophobic compounds in ligand exchange processes. The CdTe QDs capped with an amphiphilic polymer show unique properties including high water solubility, small size (average particle size of 10.5 and 14.5 nm), high quantum yields up to 44 and 49%, strong stability toward a wide pH range (pH 3-11), and excellent stability across ionic strength effect (0-1 M NaCl). Amphiphilic polymers are used here as a stable bidentate thiol motif to the CdTe QD surface. Polyethylene glycol chain was employed to promote water solubility. The amphiphilic polymers synthesized in this work were characterized by FT-IR and 1H-NMR and their QDs were also delineated by FT-IR, SEM, TEM, UV-Vis, and XRD techniques. Using fluorescence method, CMC values of Al-PEG1000(SH)$_2$ and Al-PEG2000(SH)$_2$ was 1.99 x 10^{-4} M and 7.94 x 10^{-4} M, respectively. This kind of QD was used as a fluorescent sensor for detecting ibuprofen (IBP) based on the interactions between IBP and functionalized QDs. The quenching effect on the fluorescence intensity of the sensor offered acceptable linearity with IBP concentrations in the range of 1−40 μM, with a detection limit of 0.032 μM. The sensor presented promising selectivity to IBP and was successfully applied for detecting the IBP in urine samples, and the recovered percent of IBP ranged from 93.8 to 104.0%. The obtained results provided a cheap and ultrasensitive fluorescent sensor for the fast estimation of IBP. Keywords: alginic biopolymer, CdTe, CMC, fluorescent sensor, ibuprofen, amphiphilic

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-597**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile synthesis of $ZnBi_2O_4$-C_3N_4 hybrid material with high photocatalytic activity under visible light for the removal of rhodamine B

Chu Thi Bich Thao B.T.Huy 이용일*

창원대학교 화학과

Recently, there are a lot of photocatalyst compound, one of a candidate well-known is carbon nitride (g-C_3N_4), which is a metal-free polymer semiconductor and can be synthesized by a simple heating urea, melamine or cyanmide. On other hand, the cost of C_3N_4 is cheap, easy to prepare. Besides that C_3N_4 has band gap of 2.7 eV can absorb visible light or can combine with other materials for increasing ability absorb light. Especially, it is very stable in acid, or base neutral environment. Based on its specific properties, we expect a hybrid material between $ZnBiO_4$ and C_3N_4 possess good photocatalytic property. The $ZnBi_2O_4$-C_3N_4 hybrids photocatalyst material was successfully synthesized through co-precipitation. The prepared hybrid material exhibited high photocatalytic activity for rhodamin B under visible light irradiation Hybrid C_3N_4 semiconductor material with $ZnBi_2O_4$ show to decrease by-product for the removal of RhB of $ZnBi_2O_4$ sample. $ZnBi_2O_4$/ 30% C_3N_4 exhibited a high photocatalytic activity after 3h under visible light.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-598**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Formation of Patterned Quantum Dot Composites using Thiol-Ene Click Chemistry and Imprinting Lithography

방진혁 김충현 박명환*

삼육대학교 화학과

The patterning of quantum dot (QD)-polymer nanocomposites with the unique optical and electrical properties into large area with an organized array is of great importance for various applications with photonic and optoelectronic devices. Here, we have fabricated a patterned QD-polymer composite with high photoluminescence (PL) using a thiol-ene reaction and imprinting technology. In our system, the positive charge onto QDs enhance dispersion interaction between QDs and the allylic groups on the positive charge enables QDs to chemically and strongly bind to a polymer matrix. The phenomenon was confirmed using two control QDs; neutral QDs (QD-TOH), and positive QDs without allylic groups (QD-TTMA). This synergetic effect of the charge repulsion and chemical binding in our system provides high PL with robustness. Additionally, the PL intensity shows a linear relationship with the content of QDs in a polymer matrix, indicating that the system is able to control easily a light power as a light-emitting source. These QD-polymer composites that are well-dispersed and stably fixed in a polymer matrix might provide the potential to enhance PL quantum yields in various systems with photonic and optoelectronic devices.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-599**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Visible Light Photocatalyst based on Hematite with 1-D Structures for Decomposition of Organic Contaminants in Water

이지환 곽승엽*

서울대학교 재료공학부

Organic contaminants such as phenolic compounds and chlorinated compounds become serious problem threatening human health and ecosystem integrity. Simple and effective methods are presented here to prepare visible light photocatalyst by synthesis of hematite with 1-D structures (1-D α-Fe_2O_3) for the decomposition of organic contaminants in water. Visible light photocatalyst based on 1-D α-Fe_2O_3 is capable of decomposing organic contaminants by utilizing visible spectrum containing about 45% of the solar energy. The properties of 1-D α-Fe_2O_3 were characterized via FT-IR, WXRD, FE–SEM, HR-TEM. Its magnetic property was also evaluated by VSM. The photocatalytic activity of 1-D α-Fe_2O_3 for methylene blue as a model compound was measured by UV-vis. spectroscopy. Therefore, these results suggest that 1-D α-Fe_2O_3 has a great potential for efficient visible light photocatalyst for the decomposition of organic contaminants in water.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-600**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Functionalization of Lanthanides-doped Upconversion Nanoparticles for Bioimaging

SHARIPOV MIRKOMIL Chu Thi Bich Thao B.T.Huy 이용일*

창원대학교 화학과

Rare-earth upconversion nanoparticles (UCNPs) receiving the tremendous attention of researchers last decades due to their potential application as biological luminescent labels for bioimaging application. UCNPs are considered to be very promising NIR imaging agents with the characteristics of high signal-to-noise contrast, high penetration depth and minimum photo-damage to biological system compared with conventional fluorophores. Thus, Novel UCNPs YVO_4: Yb^{3+}, Eu^{3+}, Er^{3+} were synthesized by hydrothermal method using melamine-formaldehyde as template. Surface modification of UCNPs to be hydrophilic and biocompatible were attended by Glutathione (GSH) and (3-aminopropyl)triethoxysilane (APTES).To investigate feasible applications in bio-imaging, HeLa cells were grown in DMEM (Dulbecco's modified Eagle medium) supplemented with L-glutamine, 10% FBS (fetal bovine serum) and 5mL of Pen/Strep (10.000μg/mL, 10.000 units/mL) at 37 ^{0}C and 5% CO_2. HeLa cells treated with functionalized UCNP have been wrapped by UCNP after 1h of incubation at 37 ^{0}C and 5% CO_2. Cell irradiated by NIR (980nm) showed good bio-imaging results. Moreover, cytotoxicity test showed that UCNP coated with GSH were less toxic for HeLa cells. While UCNP functionalized with APTES were more toxic, with 60% cell viability. These results establish that UCNP coated with GSH have prominent potential applications as luminescent bioimaging agents of HeLa cancer cells.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-601**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile preparation and mechanical behaviors of carbon nanotubes-reinforced carboxymethyl cellulose nanocomposites

손영래 박수진*

인하대학교 화학과

Sodium carboxymethyl cellulose/carbon nanotubes (CMC/CNT) nanocomposite films were fabricated by a simple solution casting method. The CNT can be homogeneously dispersed in water with a small quantity of CMC and was used as reinforcement into CMC polymer matrix. The crystal structure and morphologies of pure CMC, pristine CNT, and CMC/CNT nanocomposite films were investigated by using X-ray diffraction (XRD) and scanning electron microscope (SEM), respectively. The mechanical behaviors of pure CMC and CMC/CNT nanocomposite films were measured by universal testing machine (UTM). As a result, the tensile strength and Young's modulus of CMC/CNT nanocomposite films were improved according to the CNT amounts.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-602**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A simple determination of dopamine based on dithiol modified upconversion nanoparticles

정다솜 GerelkhuuZayakhuu 이용일*

창원대학교 화학과

Upconversion nanoparticles (UCNPs), that convert near-infrared (NIR) radiation to visible, have been used biological field. Furthermore, NIR irradiation has deeper penetration properties and less harmful to biological samples compared to UV excitation. Dopamine (DA) is important catecholamine neurotransmitters in nervous system. If there is any problem in the regulation of dopamine, it result various diseases for people such as bipolar disorder, depressive disorder and Parkinson's disease etc. So, it is very crucial to quantify and analyze in determination of dopamine. A simple fluorescence sensor based on fluorescent quenching effect was developed for DA determination using upconversion nanoparticles, which was modified with dithiol group (UCNPs-DT). The bond between UCNPs-DT group and DA is hydrogen bonding. The results show that the color of solution of UCNPs-DT and DA changed by binding between poly-DA and UCNPs through DT group from white to dark gray. This sensor exhibits a limit of detection as low as 20 nM for detecting DA.The UCNPs- Yb^{3+},Er^{3+}-doped $NaLuGdF_4$- was prepared using thermal method. The prepared UCNPs exhibited strong green and red emission under a laser excitation at a wavelength of 980 nm. UCNPs-DT sample was characterized by photoluminescence (PL), Field emission scanning electron microscope (FE-SEM), Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD) and transmission electron microscope (TEM).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-603**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

In vitro cell imaging using $NaLuGdF_4$:Yb^{3+}/Er^{3+}(Tm^{3+}) upconversion nanoparticles synthesized by a one-step hydrothermal method

GerelkhuuZayakhuu 정종원 **SHARIPOV MIRKOMIL** 이용일*

창원대학교 화학과

Upconversion nanoparticles (UCNPs) are a unique type of photoluminescence in which lower-energy excitation is converted into higher-energy emission via multi-photon absorption processes. In this work, a facile synthesis of Yb^{3+}/Er^{3+} (green) or Yb^{3+}/Tm^{3+} (blue)-doped $NaLuGdF_4$ UCNPs coated with malonic acid (MA) was accomplished by the one-step hydrothermal method. The UCNPs capped with the carboxylic group (-COOH) of MA on the surface to promote water solubility. The visible green (522 and 542 nm) and red (655 nm) emissions are observed from the UCNPs upon near-infrared (NIR) excitation. The successful synthesis of $NaLuGdF_4$:Yb^{3+}/Er^{3+}(Tm^{3+}) capped MA was characterized by photoluminescence (PL), field emission scanning electron microscope (FESEM), Fourier-transform infrared spectroscopy (FT-IR) and X-ray diffraction (XRD). From the obtained results, could be concluded that $NaLuGdF_4$:Yb^{3+}/Er^{3+} UCNPs capped MA was successfully synthesized by the one-step hydrothermal approach with the spherical uniform size or ~50 nm. Moreover, the carboxyl-functionalized $NaLuGdF_4$:Yb^{3+}/Er^{3+}(Tm^{3+}) UCNPs showed relatively high cell viability. The high-quality of the synthesized UCNPs have prominent potential applications for optical nanodevices and bioanalytic sensing.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-604**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Characterization of Ag-In-S-Zn and Cu-In-S-Zn alloyed quantum dot based white down conversion LED in terms of TM-30

윤희창 고민지 유희연 도영락[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

We fabricated and characterized the Ag-In-S-Zn (AISZ) and Cu-In-S-Zn (CISZ) alloyed quantum dots (QDs)-based down converted light-emitting diode (DC-LED) considering TM-30 index. The AISZ and CISZ are obtained using hot injection method. The wide band-widths and moderate quantum yields of AISZ and CISZ are recorded as 81 nm, 106 nm, and 61%, 53%, respectively, which are suitable for lighting application. To realize the AISZ and CISZ QDs based white DC-LED, we utilized the silicon binder and InGaN blue LED as blue excitation source. The visual efficiency and color performance can be characterized using TM-30, color rendering index (CRI, R_a), color fidelity index (CFI, R_f), special CRI for strong red (R_9), and luminous efficacy (LE) through measuring the optical properties of tri-color white LED. We analyzed the PL spectra of AISZ and CISZ QDs through the photoluminescence (PL) spectrophotometer, and the morphology and crystal structure information through the X-ray diffraction (XRD) and transmission electron microscope (TEM). Finally, the obtained AISZ and CISZ QD-based white DC-LED were characterized by an electroluminescence (EL) spectrophotometer.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-605**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Comparison of optical properties both three colored and six colored multi-package white LED with cesium lead halide quantum dot

이소영 윤희창 강혜림 도영락[1,*]

국민대학교 화학과 [1]국민대학교 생명나노화학과

We fabricated the cesium lead halide ($CsPbX_3$; X=Br, I) based three colored and six colored monochromatic down converted (DC) light-emitting diode (LED) and realized multi-package white LEDs to compare to their optical properties including TM-30 color standard which indicates the correct evaluations of the color rendition. The visible-emissive, narrow band-width, and highly efficient cesium lead halide ($CsPbX_3$; X=Br, I) quantum dots (QDs) were synthesized via a colloidal hot injection method. The emission wavelength and the quantum yields (QY) of $CsPbX_3$ QDs can be tuned from 490 nm to 640 nm and from 50% to 90%, respectively with 20 nm to 50 nm of narrow band-widths. To fabricate monochromatic DC-LED with $CsPbX_3$ QDs, we used UV-curable binder, InGaN blue LED chip, and long-wavelength pass dichroic filter (LPDF) which can pass the long wavelength and reflect the short wavelength. The fabricated red (R) and green (G) colored monochromatic DC-LED and a InGaN blue (B) LED can be realized RGB three color multi-package white LED with 60 mA of total current.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-606**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and Characterization of Water-glass Based Hydrophobic Silica Aerogel by Sol-gel Method

장수관 문한준 배재영*

계명대학교 화학과

Silica aerogel beads were synthesized by sol-gel method of sodium silicate as a silica precursor and using cation exchange resin filter under room temperature. The gel beads were prepared by dropwise method. A mixed solution of trimethylchlorosilane/hexane was used for solvent exchange and surface modification to be hydrophobic. The synthesized products were analyzed various method such as Brunauer-Emmett-Teller (BET) analysis, Fourier transform infrared spectroscopy (FTIR) and Optical microscope. The silica aerogel beads showed that the pore size of 12.508 ㎚, BET surface area of 487 m2/g, pore volume of 2.968 cc/g, respectively. They also displayed hydrophobic effect due to silylation as revealed by FTIR.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-607**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Facile Synthesizing method of Structure Controllable Polysilsesquioxanes with Various Silane Precursor

이종탁 이재영 배재영*

계명대학교 화학과

Laddder and cage structure polysilsesquioxanes (PSSQs) were synthesized with various silane precursor at room temperature. Structure controllable PSSQs were synthesized through controlled water condensation at sol-gel reaction of various silane precusor. Water condensation of silane reaction is more increased, PSSQs structure become cyclic structure, and water condensation is more decreased, PSSQs structure become linear resin structure. Two different PSSQs structures analysis of the obtained PSSQs are characterized using 29Si-NMR, XRD, SAXS and GPC. Well-bonded siloxane group is confirmed by T2 and T3 peak of 29Si-NMR and through XRD is confirmed more precisely the cage and ladder structures.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-608**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Dispersion of carbon black particles through surface modification using phenyl radical polymer

김민기 이승호*

한남대학교 화학과

Carbon black (CB) has relatively high strength and electrical conductivity, and is widely used in various products including ink, rubber, and paint. CB powder is generally produced in diameters of 1~5 ㎛. The carbon black particles are surface-active that easily aggregated by cohesion. This application of CB generally requires uniform dispersion of the CB particles.In this study, phenyl radical (PR) polymer with high thermal stability was synthesized by phenyl radical reaction, and then was used for surface modification of CB particles. The polymers are chemically grafted on the surface of CB particles, promoting dispersion of CB particles. The presence of PR-polymers on the surface of CB particles was confirmed using fourier transform infrared spectroscopy (FT-IR). The CB particle size and its distribution were analyzed using dynamic light scattering (DLS). The effect of the content of PR-polymer on thermal and storage stability of CB dispersions was also investigated.It was found that the aggregation tendency increases as the viscosity and pH of the CB dispersion increases. Results indicate that surface modification of CB particles with PR-polymer yields uniform CB dispersion with high thermal stability.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-609**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of dispersant structure on carbon black dispersion

배지현 이승호*

한남대학교 화학과

Carbon black (CB) has an excellent chemical strength, electric conductivity and other outstanding properties that is widely used in chemical industries: semiconductors, tires, rubber, ink, paint, toner and resin. Dispersants are often used either to break up the CB aggregates or to modify the surface of the CB particles to improve the dispersibility of CB particles. Dispersants are surfactants or zwitter ionic polymers that are soluble in water which act as steric stabilizers. CB's relatively low thermal stability limits its applications in industries that require thermal processing. Thus a polymer resin that is stable in heat is in need. In this study, phenyl radical (PR) polymer that has high thermal stability was synthesized by phenyl radical reaction. The PR-polymer created a strong covalent bond with CB particles that yielded a thermostable CB dispersion. The dispersibility and thermal stability of CB treated with PR-polymer aromatic ring-OH structure was superior than that treated with aromatic ring-COOH.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-610**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Production of Graphite Oxide and Oxidized Carbon Nitride nanodot Composite and Their Photocatlytic Performances

온새롬 박성진[1,*]

인하대학교 화학.화공융합학과 [1]인하대학교 화학과

Graphite Oxide and Oxidized Carbon Nitride nanodot Composite is a novel metal-free composite (GN). Chemical and morphological characterizations reveal that GN contains amain component of GO withwell-dispersed 2D OCN nanodots. GN shows enhanced photocatalytic performance for degrading an organic pollutant, Rhodamine B, under visible light.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-611**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Chemical structures and electrocatalytic performances of heteroatom-containing functionalities in N-doped reduced graphene oxides

심연준 오정훈 박성진*

인하대학교 화학과

N-doped graphene-based materials are excellent promising metal-free electrocatalysts for the oxygen reduction reaction (ORR). Because the N-doped graphene-based materials contain significant amounts of N and O functional groups, it is important to understand the correlation between the chemical environments of these atoms and the catalytic performance of these materials. In this work, we prepared ammonia-reduced graphene oxide (A-rG-O) using a solution-based process and a series of A-rG-O samples thermally treated at high temperatures (300–700 ℃). We investigated the chemical structure of the as-prepared A-rG-O using solid-state nuclear magnetic resonance spectroscopy of ^{15}N-labeled samples, and X-ray photoelectron spectroscopy, revealing the presence of pyridine, pyrrole and imidazole functional groups, as well as C-O and C=O groups in the rG-O network. Thermal treatment of the A-rG-O removed the N- and O-containing species, which are the catalytically active sites for the ORR. As a result overall electrocatalytic ORR performance diminished in terms of on-set and half-wave potentials, current density, and four-electron selectivity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-612**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Change of optical and photocatalytic properties of graphite oxide by exfoliation method

오정훈 박성진*

인하대학교 화학과

We propose easy exfoliation method to make a thickness-controlled graphite oxide (GO) as a metal-free photocatalyst, which is produced by stirring and sonication. All GO samples exhibit photocatalytic activity for degrading an organic pollutant, RhB under visible light, and the thickest sample shows the best catalytic activity. UV-vis-NIR diffuse reflectance absorption spectra indicate that thicker GO samples absorb more vis-NIR light than thinner ones. Density-functional theory calculations show that graphite oxide has a much smaller band gap than that of single-layer graphene oxide, and thus suggest that the largely-reduced band gap is responsible for this trend of light absorption.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **MAT.P-613**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 11:00~12:30

N-doped reduced graphene oxides with anchored iridium compound as using oxygen reduction reaction catalyst

신윤석 박성진*

인하대학교 화학과

Many researches studied new system with high catalytic performance in the oxygen reduction reaction(ORR) for available application in fuel cells. Our team develop a on-pot solution process for producing a novel hybrid material. The hybrid consisting of Ir species anchored on N-doped graphene oxide is synthesized by reacting N-doped graphene oxide with IrCl3 centerdot xH2O in dimethylformamide under reflux. The hybrid shows high long-term duarability, good tolerance for methanol poisoning and high electrocatalytic performance for the ORR in alkaline media with an onset potential of 0.88 V (versus the reversible hydrogen electrode)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-614**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Organometallic catalyst with N-doped graphene complex : Implications for oxygen reduction reaction reactivity of organometallic Co-O_4-N-species

박성희 박성진[1,*]

인하대학교 화학화공융합대학원 [1]인하대학교 화학과

Organometallic complexes with graphene-based materials can give rise to enhanced catalytic performance. It is important to understand the chemical structures within hybrid materials. In this work, archetypical hybrid materials are synthesized by the reaction of an organometallic complex, [CoII(acac)2] (acac = acetylacetonate), with N-doped graphene-based materials at room temperature. Experimental characterization of the hybrid materials and theoretical calculations reveal that the organometallic cobalt-containing species is coordinated to heterocyclic groups in N-doped graphene as well as to its parental acac ligands. The hybrid material shows high electrocatalytic activity for the oxygen reduction reaction (ORR) in alkaline media, and superior durability and methanol tolerance to a Pt/C catalyst. Based on the chemical structures and ORR experiments, the catalytically active species is identified as a Co-O4-N structure.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-615**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Effect of oxygen level on capacity and cyclic performance of reduced graphene oxide in Lithium-ion batteries

김수진 박성진[1,*]

인하대학교 화학/화학공학 융합 [1]인하대학교 화학과

Graphene-based materials are expected to be advanced anodes for achieving high energy and power densities in Lithium-ion batteries (LIBs). In spite of intensive research on reduced graphene oxide (rG-O) on this aspect, few have explained the relationship between LIB performance and the degree of reduction of graphene oxide. In this work, we report the performance of LIB anodes using rG-O materials with different oxygen levels. A series of rG-O samples is produced by refluxing an aqueous graphene oxide suspension for different times. The C/O ratios of the rG-O sample are found to increase gradually from approximately 1 to 6, with no heteroatoms other than oxygen atoms. The rG-O sample with the lowest oxygen level delivers the highest anodic capacity and good durability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-616**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

The results of KOH Processing on the Chemical Structure and Electrocatalytic Activity of Reduced Graphene Oxide Materials

장다운 박성진[1,*]

인하대학교 자연과학부/화학과 [1] 인하대학교 화학과

Reduced graphene oxide (rG-O)-based materials have great efficient metal-free electrocatalysts for the oxygen reduction reaction (ORR) because of their electrical and electrochemical properties and large surface area. Long term durability and chemical stability of the catalysts in the presence of electrolytes such as aqueous KOH solution are important for their use in practical applications. In this study, three types of rG-O and rG-O-K (rG-O after reaction with KOH) materials were synthesized. The synthesized rG-O-K was compared with chemical structures, surface areas, and catalytic ORR performances those of the corresponding rG-O materials. The onset potentials of the rG-O materials for electrocatalytic reduction of oxygen are almost the same as those of the corresponding rG-O-K materials; however, the current density and the number of transferred electrons are significantly reduced. These data show that the catalytic ORR performance of rG-O-based materials can be altered by KOH.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-617**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

pH-Responsive DNA-Driven Au Nanomachine for Combinational Cancer Therapeutics

박형목 김진환 김원종*

POSTECH 화학과

Owing to the sequence specific hybridization, DNA has attracted enormous attention as a programmable and predictable building block for dynamic nanomachine. We present herein a pH-responsive multifunctional Au nanomachine operated by functional DNA for combined chemo-, phototheraml, and photodynamic therapy. To achieve that, pH-responsive DNA sequence, known as i-motif, was grafted on the surface of gold nanoparticle by gold-thiol interaction. By employing the fact that the anticancer drug, doxorubicin (DOX), easily intercalates on duplex DNA, the Au nanomachine was exploited for DOX delivery carrier. Once this nanoparticle is internalized into the cells, endosomal acidic pH induces the dehybridization of i-motif and its complementary sequence, and subsequently DOX was released from duplex structure. Because i-motif DNAs on the gold nanoparticle bind to nearby i-motif DNAs on another one, gold nanoparticles were aggregated to bigger particles, which enable the photothermal therapy when NIR light was subjected. As well, a photosensitizer was selectively loaded on the specific DNA sequence for photodynamic therapy. Taken all together, combinatorial effect of chemo-, photothermal, and photodynamic therapy was evaluated at the cellular level in a synergistic manner. The dynamic nanomachine developed herein would provide a simple way to design a combinational cancer therapeutic system.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-618**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

A new approach to synthesize composition-controlled PtPd alloy nanocatalysts supported on graphene and their enhanced electrocatalytic peformances

예성지 김영윤 박오옥*

KAIST 생명화학공학과

Uniformly dispersed PtPd alloy nanocatalysts supported on graphene are one of the prospective electrocatalysts in methanol oxidation reaction. Here, we report a new and simple approach for synthesizing uniformly dispersed PtPd alloy nanocatalysts supported on graphene nanoplatelets (GNPs) (PtPd-GNPs) by introducing bifunctional material which can be used to modify the GNP surface and simultaneously reduce metal ions. As bifunctional materials, poly(4-styrenesulfonic acid) (PSS), poly(vinyl pyrrollidone) (PVP) and Nafion could be used and the synthesis steps were minimized comparing to previous reports thanks to their dual roles. The as-prepared nanocatalysts on GNP clearly exhibit a PtPd alloy structure with uniform size around 2 nm and strongly anchored with well-distributed states. Moreover, the Pt/Pd atomic ratio and loading density of PtPd-GNPs can also be easily controlled by changing the feed ratio between metal precursors and by changing the mass ratio of GNP to metal precursor, respectively. The readily prepared PtPd-GNPs shows composition-dependent electrocatalytic activity and stability in methanol electrooxidation reaction. Especially, PtPd-GNP with 60 at. % of Pt exhibits the highest electrocatalytic activity and stability among the samples, which is also much higher than monometallic Pt-GNP.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-619**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Single-Crystal Heterojunction Organic Nanowires for High-Integrated Organic Electronics

박경선 성명모*

한양대학교 화학과

High-quality organic single-crystal nanowires were used for the fabrication of high-integrated organic electronic and optoelectronic devices. Direct printing processes including inkjet printing and transfer printing were employed for producing single-crystal heterojunction organic nanowires which were simultaneously synthesized, aligned, and patterned to specific positions on substrates. The direct printing method allows two- or three-dimensional heterogeneous integration of different functional organic materials, e.g. lateral/vertical heterojunction nanowires. Organic p-n heterojunction diodes produced by using an appropriate configuration of organic nanowires were characterized as a fundamental electronic component for high-integrated organic electronics.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-620**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fabrication of Nickel Sulfide(NiS) Thin Films using Atomic Layer Deposition as Low Cost Counter Electrodes for Pt-Free Dye-Sensitized Solar Cells

정진원 김홍범[1] 성명모[1,*]

한양대학교 자연과학대학 화학과 [1]한양대학교 화학과

Dye-sensitized solar cells (DSCs) are promising candidates for light-to-energy conversion devices due to their low-cost, easy fabrication and relative high conversion efficiency. An important component of DSCs is counter electrode (CE) collect electrons from extrernal circuit and reduct I3- to I-. The conventional CEs are thermally decomposed Pt on fluorine-doped tin oxide (FTO) glass substrates, which have shown excellent performance and stability. However, Pt is not suitable in terms of cost effect. In this report, we demonstrated that nickel sulfide thin films by atomic layer deposition (ALD)-using Nickel(1-dimethylamino-2-methyl-2-butanolate)2 and hydrogen sulfide at low temperatures of 90-200 °C—could be good CEs in DSCs. Notably, ALD allows the thin films to grow with good reproducibility, precise thickness control and excellent conformality at the angstrom or monolayer level. The nickel sulfide films were characterized using X-ray photoelectron spectroscopy, scanning electron microscopy, X-ray diffraction, hall measurements and cyclic voltammetry. The ALD grown nickel sulfide thin films showed high catalytic activity for the reduction of I3- to I- in DSC. The DSCs with the ALD-grown nickel sulfide thin films as CEs showed the solar cell efficiency of 7.12% which is comparable to that of the DSC with conventional Pt coated counter electrode (7.63%).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-621**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Self-Assembly of Eutectic Liquids with Nanosurfaces

정기범 이승현[1,*] 박치영[2,*]

한국과학기술연구원(KIST) 탄소융합소재 [1]수원대학교 신소재공학과 [2]한국과학기술연구원 (KIST) 탄소융합소재연구센터

본 연구는 공융액체(eutectic liquid)가 나노 단위의 계면에서 자기 조립되는 현상을 제어하고, 탄화 특성을 연구하였다. 상온에서 액체 상태인 공융액체는 탄소나노튜브나 무기재료 표면에서 자기조립이 유도되어 gel 로 변하는 거동을 보였다. 이를 rheometer, XRD 등을 이용하여 분석하였고, rheology 결과는 이 gel 이 semi-solid 임을 증명하였다. 또한 이 재료들의 탄화 조건을 제어함으로써 새로운 다공성 재료 및 전기 촉매 응용에 관하여 논하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-622**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Ceramic Coating of Chlorine Method Rutile TiO_2 for White Pigments

유리 윤지연[1] 김유진[*]

한국세라믹기술원 엔지니어링세라믹센터 [1]한국세라믹기술원 엔지니어링 세라믹 센터

Titanium dioxide (TiO_2) is used as a white pigment for architecture, cosmetic, and paint because it efficiently scatters visible light, there by imparting whiteness, brightness and opacity. This work describes a means of improving the whiteness and reflectivity of ceramic coated TiO_2 pigment. To retain and enhance the properties of white pigment, we adopted core-shell system with the silica (SiO_2), aluminum oxide (Al_2O_3) and zirconium dioxide (ZrO_2) as shell materials. These inorganic surface treatments provide improvements in important performance properties such as dispersibility in water and in a range of organic liquids, hiding power efficiency, chalk resistance, and resistance to discoloration by photo-reduction. Control of the shell thickness and whiteness of the TiO_2 pigment was important factor for high quality outdoor white pigments and their shell thickness was achieved by regulating the reaction time, concentration and shell materials.Details of the coloration and phase structure of TiO_2 pigment were characterized by UV-vis, CIE Lab color parameter measurements, TEM (transmission electron microscopy) and XRD (powder X-ray diffraction).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-623**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Development of inkjet-assisted nanotransfer printing for fabrication of organic integrated circuits

백장미 박경선 성명모*

한양대학교 화학과

For manufacturing of high-performance organic electronic circuits, effective heterogeneous integration of different nanoscale organic materials is required. Herein, we report a new direct printing method which enables monolithic integration of crystalline nanowire arrays with a various organic materials. This direct printing technique, referred to as “inkjet-assisted nanotransfer printing (inkjet-NTP)”, is combined inkjet printing and nanotransfer printing via a liquid-bridge-mediated transfer process. In this method, we introduce a new concept of an assembled mould, a universal mould, which contains simple nanoline patterns but, in combination with inkjet printing, can produce a large-scale integration of various nanopatterns with multiple kinds of organic nanowires. The morphology of individual organic nanowires and mutual alignment between them can be controlled as desired with control of ink droplet size, ink droplet number and ink deposition locations as well as the nanoline patterns in the mould. The Inkjet-NTP was utilized to fabricate wafer-scale organic electronic circuits composed of field-effect transistors (FETs) and complementary inverters and p-n diodes, demonstrating its capability to produce a high-performance multifunctional organic device.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-624**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fabrication of nanostructured vanadium oxide thin film for smart window applications

정유홍 정성욱[1,*]

부산대학교 화학공학과 [1]부산대학교 화공생명공학부

Vanadium dioxide (VO2) has attracted much attention because it is known to undergo a reversible, thermally induced metal semiconductor phase transition. The outcome of this phase transition is non-linear optical, electrical and magnetic characteristics with respect to temperature. Particularly its optical properties change significantly in the visible and near IR range at its phase transition temperature (TC ~ 68℃). As the temperature exceeds TC, it goes through structural change and becomes less transparent and more reflective, preventing thermal radiation from excessively heating while remaining visually transparent. Therefore, this phenomenon can be applicable to smart window applications because incorporating economically sustainable thermochromic films into window products could have significant impact on energy saving technology.We developed solution-phase synthetic routes to monodisperse, organically functionalized vanadium oxide nanoparticles in order to use them as potential thermochromic materials for smart window application. Vanadium oxide thin films have been fabricated via spin coating the solution of vanadium oxide nanoparticles. As-prepared vanadium oxide nanoparticles and their thin film have been characterized by means of transmission electron microscopy (TEM), scanning electron microscopy (SEM), powder X-ray diffraction (XRD), Fourier transform infrared absorption spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS). Results of structural and spectroscopic studies on the formation of vanadium oxide nanoparticles and their films as well as the effects of solution compositions and reaction conditions will be discussed together with the optical properties of vanadium oxide thin films.

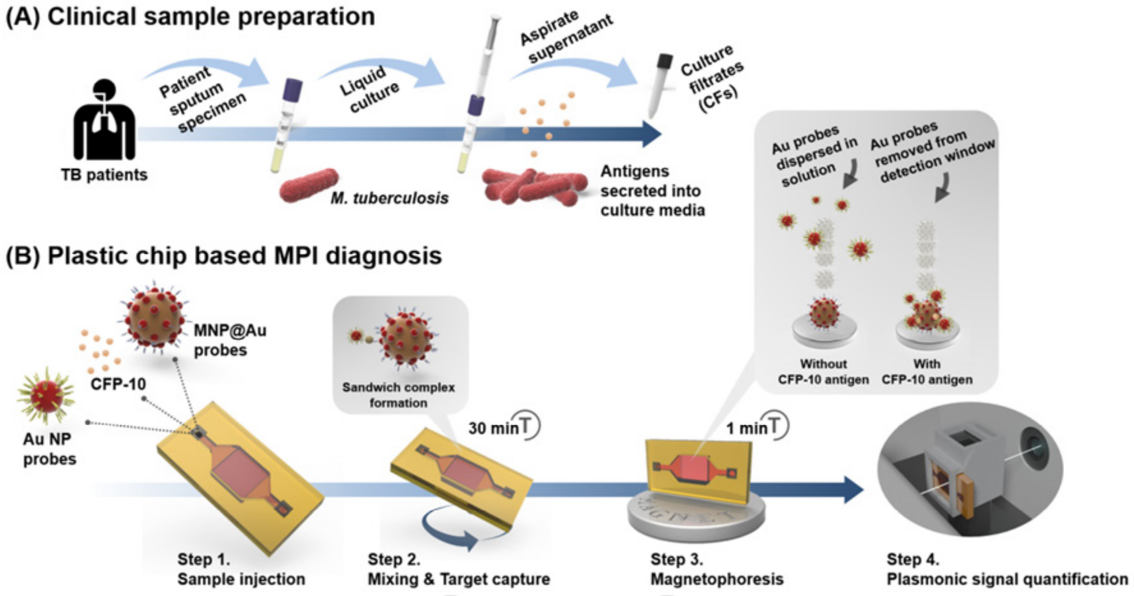
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-625**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Clinical serodiagnosis of tuberculosis using plastic chip based magnetophoretic immunoassay

김정효 오상진[1] 정기재[1] 이재범[2,*]

부산대학교 인지메카트로닉스 공학과 [1]부산대학교 인지메카트로닉스공학과 [2]부산대학교 광메카트로닉스공학과

Tuberculosis (TB) remains a relevant infectious disease in the 21st century and its extermination is still far from being attained. Due to extreme infectivity of incipient TB patients, a rapid sensing system for proficient point-of-care (POC) diagnostics is required. In our study, a plastic chip−based magnetophoretic immunoassay (pcMPI) is introduced using magnetic and gold nanoparticles (NPs) modified with *Mycobacterium tuberculosis* (MTB) antibodies. This pcMPI offers an ultrasensitive limit of detection (LOD) of 1.8 pg/mL for the detection of CFP-10, an MTB-secreted antigen, as a potential TB biomarker with high specificity. In addition, by combining the plastic chip with an automated spectrophotometer setup, advantages include ease of operation, rapid time to results (1 h), and cost-effectiveness. Furthermore, the pcMPI results using clinical sputum culture filtrate samples are competitively compared with and integrated clinical data collected from conventional tools such as the acid-fast bacilli (AFB) test, mycobacteria growth indicator tube (MGIT), polymerase chain reaction (PCR), and physiological results. CFP-10 concentrations were consistently higher in patients diagnosed with MTB infection than those seen in patients infected with non-tuberculosis mycobacteria (NTM) ($P < 0.05$), and this novel test can distinguish MTB and NTM while MGIT cannot. All these results indicate that this pcMPI has the potential to become a new commercial TB diagnostic POC platform in view of its sensitivity, portability, and affordability.


(A) Clinical sample preparation
TB patients
Patient sputum specimen
Liquid culture
M. tuberculosis
Aspirate supernatant
Antigens secreted into culture media
Culture filtrates (CFs)
(B) Plastic chip based MPI diagnosis
MNP@Au probes
CFP-10
Au NP probes
Sandwich complex formation
30 min
1 min
Au probes dispersed in solution
Au probes removed from detection window
Without CFP-10 antigen
With CFP-10 antigen
Step 1. Sample injection
Step 2. Mixing & Target capture
Step 3. Magnetophoresis
Step 4. Plasmonic signal quantification

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-626**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Organic-inorganic nano-laminate for gas diffusion barrier by molecular layer deposition and atomic layer deposition

윤관혁 성명모*

한양대학교 화학과

Organic light-emitting diodes (OLEDs) are the attractive candidates for the flexible electronics. However, being extremely sensitive to air and moisture, the OLED based-devices should be encapsulated with transparent barrier film having ultra-low water vapor permeability. The present work reports a novel barrier thin film consisting of alternative layers of self-assembled organic layer and alumina exhibiting high mechanical flexibility and ultra-low water vapor permeability. The barrier films are deposited using the combined molecular layer deposition and atomic layer deposition technique at the same reaction chamber at 80 °C to obtain homogeneous and conformal coating to a large area. The barrier performance of the gas-diffusion barrier was determined by Ca conductance and Ca dot array tests. At optimized thickness ratio of 1:2 for the SAOLs/Al_2O_3 nano-laminate film with total 100 nm thickness of the Al_2O_3 layer, the barrier film demonstrates the ultra-low water vapor transmission rate of 2.99×10^{-7} g/m^2day, which is the lowest permeability achieved by the thin and transparent gas-diffusion barriers reported so far. Based on the outstanding barrier properties with good flexibility and transparency, the nano-laminated film was applied to the commercial OLED panels as a gas-diffusion barrier film. The results indicate the enhanced durability of the panels with significant prevention on defect propagation by thin SAOLs layers.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-627**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Mg-stabilized InP/GaP/ZnS QDs for LED applications

백승민 서해운[1] 김상욱[2,*]

아주대학교 분자과학기술학과 [1]아주대학교 분자기술학과 [2]아주대학교 응용생명화학공학부

In the last few year, people have focused on study for improved quantum dots (QDs). Above all, InP-based QDs have promising materials for light emitting diode(LED). However, InP-based QDs have some critical problems, for example stability, compared with CdSe-based QDs. For improving stability, many reaserch groups have synthesized thick outer shells and has been applied for applications. We used magnesium cations for improving stability of InP/GaP/ZnS. As a result, we demonstrated very small amounts of Mg cation as surface stabilizers while the maintaining a quantum yield of QDs. Finally, We fabricated QD based LED chips. It also yielded improved values Including CRI of 84.4, CCT of 3799K, and EQE of 129.57lm/W.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-628**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Full color luminescence of InP/GaP/ZnS QDs with heating up process

권오훈 안소연 박중필 김상욱[1,*]

아주대학교 분자과학기술학과 [1]아주대학교 응용생명화학공학부

Quantum dots that are based on InP has attracted a lot of attention for use in optical applications. The quantum dots have been developed in various types that are based on InP, such as InP / ZnS, InP / ZnSe, InP / GaP / ZnS. However, the initial synthesis of hot injection could not produce the required optical properties with high reproducibility.They also could not successfully support the commercialization efforts.Here, we show how to simply synthesize the InP / GaP / ZnS through the heating up process. This reaction can be completed within 0.5h and represent a full color from blue to red. If a blue light-emitting, t-DDT was used in order to prevent particle growth. By adjusting the amount of the Myristic acid showed a color from green to orange. Using a large amount of gallium chloride leads to a red color.We produced InP/GaP/ZnS QDs of high quality by this method (blue QY: ~40%, FWHM: 50 nm; green QY: ~85%, FWHM: 41 nm; red QY: ~60%, FWHM: 65 nm). We used the t-DDT not the sulfur sources reported.Compared with n-DDT, t-DDT was more reactive, which allowed for the formation of a thicker shell.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-629**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Electrical and optical properties of Al-doped ZnO films prepared by atomic layer deposition at low temperature

방지홍 성명모*

한양대학교 화학과

Al-doped ZnO was commonly used for the transparent conducting electrodes, but it was not suitable for flexible application so far, because the high fabrication temperature was essential to achieve good electrical properties. In this study, ZnO/Al2O3 multi layers were fabricated by alternating Atomic layer deposition (ALD) on PET substrate at 120℃ using diethlyzinc (DEZ), trimethylaluminum (TMA) and deionized water with additional ultra-violet (UV) exposure. The growth rate, electrical and optical properties of the multi layers were studied with a variety of cycle ratio of ZnO and Al2O3 sub layers. The ZnO/Al2O3 multi layers deposited at 120℃ has low conductivity. However, after few minutes of .UV light exposure, the films show high conductivity. The conductivity can controlled to positive direction by increasing the UV exposure time. Furthermore, the film showed high transparency(80%) and high stability against the degradation of the electrical conductivity.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-630**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Separation of primary amine containing molecules via covalent bond using a special type of anhydride grafted silica

송영준 이연*

서울대학교 화학부

There are various organic molecules which contain amino functional group in their molecular structure because of property of nitrogen atom which can easily conjugate with other molecule via their lone pair electrons. So, purification and recognition of amine molecule what we want to separate is very important and challengeable issue. A special type of anhydride derivatives make covalent bond with primary amines under basic condition, and the formed amide acid degrade at acidic condition. In this research we synthesized and characterized a special type of anhydride grafted silica support for amine affinity column. And by this method small or large molecules which have primary amine group are successfully separated in the mixture of various functional groups i.e. alcohol, carboxylic acid, tertiary amine and quaternary ammonium groups.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-631**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Study on the correlation existing between Li^+adsorption capacity and the physical properties of spinel-type adsorbents

박윤봉

충남대학교 화학과

Spinel-type lithium manganese oxides have received considerable attention as Li^+ ion selective adsorbents. Among them, $LiCo_{0.5}Mn_{1.5}O_4$ is expected to have the optimized structure for the Li^+ selective adsorbents because $LiCo_{0.5}Mn_{1.5}O_4$ shows relatively low dissolution ratios of metal ions and good Li^+ adsorption capacity. In this study, we are quite successful in preparing homogeneous $LiCo_{0.5}Mn_{1.5}O_4$ with various morphologies. Their Li^+ adsorption capacities and specific surface areas are measured and compared to find out any correlation between the Li^+ adsorption capacities and their physical properties. The characterization of $LiCo_{0.5}Mn_{1.5}O_4$ is performed X-ray powder diffraction (XRD), inductively coupled plasma-atomic emission spectroscopy (ICP-AES), BET method and scanning electron microscope (SEM).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-632**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Role of Substrate Surface on Magnetic Field-Induced Assembly of Magnetoplasmonic Nanoparticles

TRAN VAN TAN 이재범[1,*]

부산대학교 나노융합기술 [1]부산대학교 광메카트로닉스공학과

The assembly mechanism of Au-coated Fe3O4 core–shell superparamagnetic nanoparticles (Fe3O4@Au NPs) was investigated thoroughly, revealing that besides van der Waals and magnetic dipolar forces, the hydrodynamic interactions resulted from the existence of a net repulsive force between NPs and the substrate play the fundamental role in control of nanochain structures. Magnetic force microscopy (MFM) and vibrating sample magnetometer (VSM) were used to study the magnetic properties of the MPNCs, which were compared with those of Fe3O4 nanochains. The results suggest the possibility of using such a mechanism to construct and regulate other assembled structures consisting of nanoscale building blocks as well as for further research on biomedical applications and device fabrication in nanoscale regime.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-633**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Fabrication of ZnO thin films with high conductivity and stability by UV-assisted atomic layer deposition

윤홍로 성명모*

한양대학교 화학과

Compounds of ZnO is very attractive compound semiconductors due to their wide band gap (~3.3eV) characteristics and large exciton binding energy (60meV). However, ZnO preparing by low temperature atomic layer deposition (ALD) has low conductivity. Here, we report the highly transparent, and highly conductive air-stable thin film of ZnO using ALD at low temperature under in situ UV irradiation of the growing film. X-ray photoelectron spectroscopy (XPS) was used to reveal that the UV irradiation generates oxygen vacancies, partially removes O–H bonds, and thereby improves the electrical conductivity. Thus, the in situ UV irradiated ZnO film shows an electrical resistivity of 5.5 × 10-4 Ω cm, compairing to 0.25 Ω cm resistivity of the pristine ZnO film, and an optical transparency of nearly 90%. In addition, even on prolonged exposure of the film to air, it maintains high stability and conductivity against the degradation of the electrical conductivity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-634**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Exploration of Plasmon-Mediate Photocatalysis with Au-Cu_2O Heteronanocrystals Produced by Site-Selective Growth of Cu_2O on Desired Sites of Au Nanocrystals

위대한 한상우*

KAIST 화학과

Here, we present the rational strategy for realization of plasmonic metal-semiconductor heteronanocrystals (HNCs) with intended configurations through site-selective growth of semiconductor Cu_2O at desired sites of anisotropic Au NCs. Both the exploitation of structural characteristics of Au NCs and the selective stabilization of their surfaces are keys to the construction of HNCs with a specific configuration. These HNCs can provide the opportunity to explore on plasmonic effects to photocatalysis depended on coupling manner between plasmonic NC and semiconductor. HNCs produced by Cu_2O overgrowth preferentially on the multiple high-curvature sites of Au NCs exhibited prominent photocatalytic hydrogen production activity due to efficient charge separation by strong plasmon excitation at the interconnecting junction between Au and Cu_2O and subsequent sustainable hot electron transfer from Au to Cu_2O.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-635**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Identification of catalytic active site of Pd nanoparticles in Suzuki-Miyaura coupling through site selective deposition on edge and vertex with catalytic inert Au

함경록 한상우[1,*]

KAIST 화학 [1]KAIST 화학과

We have successfully synthesized Pd rhombicdodecahedron nanoparticles (RD NPs) and structurally heterogeneous nanoparticle with Pd and Au from rational design. Edge covered Pd nanoparticles (ECP NPs) were synthesized with partially modification of Pd RD NPs' surfaces, and the catalytic active sites were observed through this elaborate modification. These NPs were used as catalysts in Suzuki coupling. Because of selective deposition of gold to the edge and vertex sites of Pd RD NPs, reactivity difference was occurred between two kinds of catalysts. This difference with physically blocked NPs could be direct evidence that edge and vertex atoms were main catalytic active sites instead of indirect evidences of past several researches. Pd RD NPs had higher reactivity compared with ECP NPs because the former had exposed edge and vertex atoms which had chemical activity because of lower coordination number. From the several experiments, the reaction pathway was turned out probably heterogeneous, and the catalysts had high recyclability in Suzuki coupling. Lastly, in previous researches about Suzuki coupling with high index facet NPs, for example, concave cube, their higher reactivity would be explained because of more numbers of catalytic active edge and vertex atoms compared with low index facet NPs. Further studies that the detailed investigation about surface modification of metal NPs were suggested, and through that kinds of studies, verification of exact chemical pathway of organic reaction with metal NPs would be necessary and important.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-636**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Enhanced Performance of Blue Polymer Light-emitting Diodes by localized surface plasmon coupling of Ag Nanoparticles introduced through Ligand-exchange Process

김영윤 박오옥*

KAIST 생명화학공학과

Utilizing localized surface plasmon resonance of metal nanoparticles (NPs) in organic light-emitting diodes have been intensively researched to improve an internal quantum efficiency. In this study, Ag NPs were synthesized through polyol process and introduced in the blue polymer light-emitting diodes (PLEDs), which have been suffered from low efficiency. In particular, Ag NPs were attached on the indium tin oxide (ITO) surface through ligand-exchange process, which guarantees well-dispersed state of Ag NPs, in order to maximize the resonant coupling and to prevent optical and electrical side effects. In addition, the mercaptoacid molecules not only acted as coupling agent between ITO and Ag NPs, but also aided to transfer holes by increasing work function of ITO, which was confirmed by measurement on hole-only devices and ultraviolet photoelectron spectroscopy. As a result, the maximum current efficiencies of blue PLEDs were improved by 25 % with thioglycolic acid (TGA) only, and enhanced by 48 % with 0.302 nM Ag NPs attached with assistance of TGA. The enhancement mechanism was confirmed as the resonant interaction between Ag NPs and blue light-emitting polymer, SPB-02T, by time-resolved photoluminescence spectra and normalized electroluminescence spectra.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-637**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Molecular Dynamic Simulations on the Mechanical Force Dependent Structures of Poly(Vinylidene Fluoride) Piezoelectric Polymer for Novel Renewable Energy Applications

유택희 Yves Lansac[1] 장윤희[2,*]

GIST 신소재공학부 [1]Université François Rabelais [2]DGIST 에너지시스템공학

Poly(vinylidene fluoride) (PVDF) is one of the best piezoelectric polymers owing to its net monomeric (CH_2CF_2) dipole moments well aligned in its β-phase crystals. Various efforts such as cold drawing, stretching, poling, copolymerization and inclusion of additives have been applied to maximize its piezoelectric coefficient by transforming the inherently-amorphous PVDF into the β-phase crystals, but the improvement has been limited due to the lack of systematic molecular-level understanding of the effect of the shear stress on the crystallization of PVDF. In the current study we therefore carry out non-equilibrium molecular dynamics simulations to virtually mimic the crystallization of amorphous PVDF under various amounts of shear stress. It is interesting to find that the β-phase crystallinity, the polarization, and the net dipole are maximized at a critical value of shear velocity rather than increasing monotonically with shear velocity. The presence of the critical shear velocity and its predicted value are in a good agreement the experimental observation (Org. Electron. 28, 67-72, 2016). Our simulations also predict a shear-induced development of various domains showing parallel, anti-parallel, and random alignments of dipoles.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-638**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Synthesis and luminescence properties of copper(I) halide melamine complexes

김주현 김재겸 강경모 김승주[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 에너지시스템학부

Copper(I) halide melamine complexes were synthesized by precipitation method. The crystal structure of CuX-melamine(X = Cl, Br, I) has a triclinic symmetry (space group = $P1$). The unit cell volume of copper(I) halide melamine complexes shows a linear increase with the size of halogen ion. This compounds exhibit an 1D chain structure grown along *c*-axis. Thermogravimetric analysis (TGA) results showed that CuX-melamine complexes have Cu : X : melamine = 1 : 1 : 1 molar ratio. In photoluminescence measurement, the excitation spectra were obtained at maximum excitation-emission wavelength of 297nm-520nm, 300nm-527nm, and 304nm-460nm for CuCl-melamine, CuBr-melamine, and CuI-melamine, respectively. The relation between the crystal structure and the luminescence property will be discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-639**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Subcellular Organelle Targeting AuNRs(gold nanorods) for Efficient Photothermal Therapy

이영주 임동권*

고려대학교 KU-KIST 융합대학원

Plasmonic metal nanoparticle is usually made of novel metal likewise gold, silver and modified by other functional materials such as peptide, DNA etc for in-vivo, in-vitro experiment. The nanostructures formatted by nanoparticle can be utilized for live cell imaging technology and anticancer technology.Gold nanorods which have a suitable aspect ratios absorbs and scatters a light of the Near-infrared region. These unique characters provide the potential of designing novel optically active reagents for continuous molecular imaging and photothermal cancer therapy. Subcellular Organelle Targeting gold nanorods are synthesized through the surface modification with targeting probe such as cell penetrating peptide, nuclear localization sequence, mitochondria localization sequence. Each Targeting gold nanorods will arrive within a different cell location and we detect the targeting distinction using dark-field image and compare photothermal effect of each other targeting gold nanorods using plate-readers.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-640**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Crystal structure and ionic conductivity of $Na_3TeGa_3P_2O_{14}$

손봉수 박용진 김성철 김승주[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 에너지시스템학부

The duggaite structure has attracted great interest in materials science due to their open-framework structure. In this work, $Na_3TeGa_3P_2O_{14}$, an isostructure with mineral dugganite, was synthesized by conventional solid state reaction and its crystal structure was characterized by powder X-ray diffraction. It crystallizes hexagonal symmetry (space group *P*321) with lattice parameters a = 8.1273(2) Å, and c = 4.9394(2) Å. This structure is built by connection of NaO_8 decahedra, TeO_6 octahedra, GaO_4 tetrahedra and PO_4 tetrahedra, which forms the large cavities. The ionic conductivity of $Na_3TeGa_3P_2O_{14}$ was measured using impedance analyzer: The ionic conductivity, σ ≈ 3.6 x 10-4 S/cm at 773K and the activation energy, Ea ≈ 0.52eV in the temperature range of 323K ~ 773K

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **MAT.P-641**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 11:00~12:30

Plasmonic engineering of ~1 nm intra-nanogap embedded nanostructures for biomedical SERS nanoprobes

오정욱 남좌민*

서울대학교 화학부

Plasmonic nanogap has been receiving extensive attention due to the extraordinary enhancement of plasmonic coupling in this very narrow region. In general, the localized surface plasmon coupling in the nanogap is greatly enhanced with the reduction of nanogap thickness. However, this trend collapses in the region of < 0.5 nm due to the quantum tunneling effect. For this reason, the synthesis of ~1 nm ultrasmall nanogap with high precision and uniformity, is particularly important for the development of ultrasensitive and quantitative SERS sensors. In recent years, we have developed ~1-nm intra-nanogap embedded gold nanoparticles (AuNPs) with nanobridges between Au core and Au shell, which produced strong (enhancement factor $>10^8$) and highly homogeneous and reproducible SERS signals. Interestingly, ~1-nm intra-nanogap inside these Au-nanobridged nanogap particles (Au-NNPs) can be controlled by sequence and grafting density of the DNA strands modified on core AuNPs, which enable to change the features of plasmonic coupling and SERS. In addition, the SERS intensity of Au surface roughness-controlled nanobridged nanogap particles (Au-RNNPs) was ~1 order greater than that of Au-NNPs with smooth surface. Our synthetic strategies and results provide useful guideline to design and synthesize plasmonic nanostructures with nanogap and utilize these structures for optics and biomedical applications.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

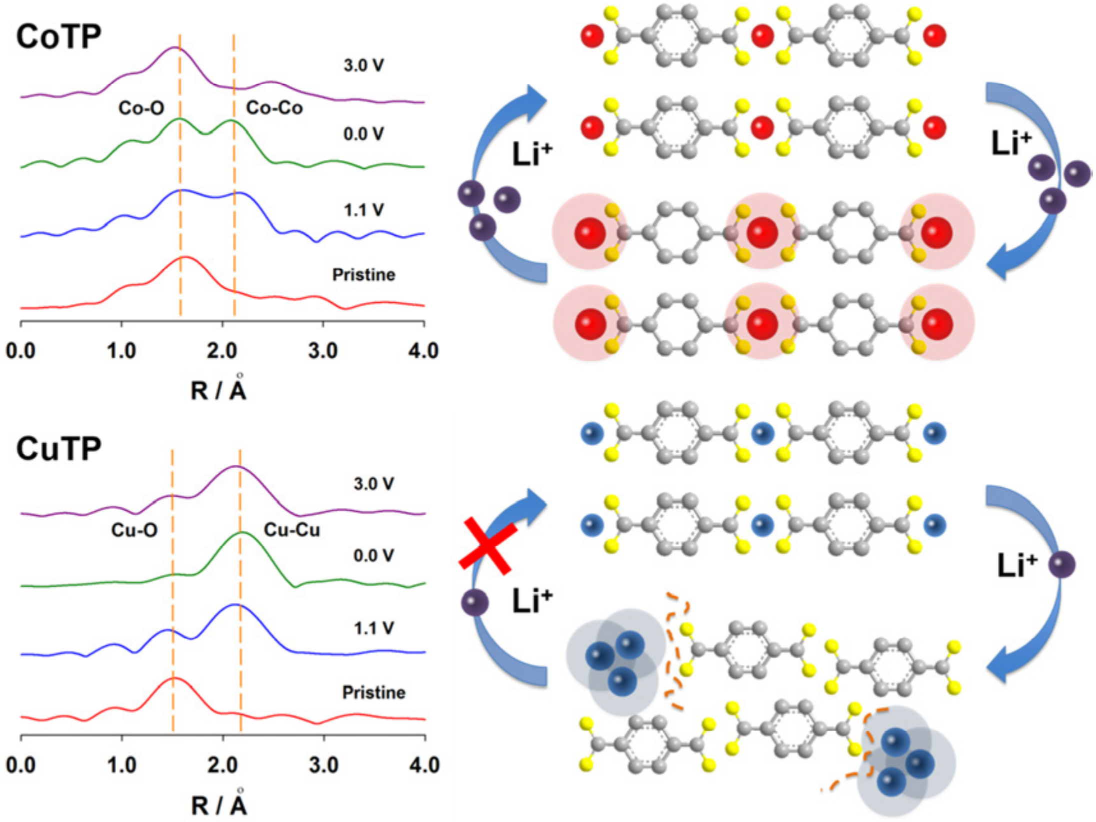
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-515**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Origin of Metal-Specific Reversible Conversion Processes for Metal-Organic Coordination Complexes in Lithium-Ion Batteries

이현호 홍성유[1,*]

UNIST 에너지및화학공학부 [1]UNIST 나노생명화학공학부

Conversion electrode materials exploiting transition-metal redox-couples are prominent candidates for high capacity lithium-ion batteries. While extensive mechanistic investigations of inorganic host materials have been conducted, little is known for redox-active metal-organic coordination complexes in the context of solid-state reversibility. Herein we disclose that metal-specific reversible conversion is governed by close spatial-proximity between metallic nanoparticles and organic ligands as verified by combined X-ray absorption spectroscopy and high-resolution transmission electron microscopy studies. Moreover, fully reduced metallic nanoparticles well-dispersed in the organic matrix offer electrically conductive paths allowing multi-electron transfer to redox-active • •conjugated molecules. We further extend coordination complex scope by synthesizing cobalt-2,5-thiophenedicarboxylate, which presents the distinctive electrochemical performance with a large reversible capacity of ~1100 mAh g-1 over 100 cycles at exceptionally high current density of 500 mA g-1.


CoTP
3.0 V
Co-O
Co-Co
0.0 V
1.1 V
Pristine
0.0
1.0
2.0
3.0
4.0
R / Å
CuTP
3.0 V
Cu-O
Cu-Cu
0.0 V
1.1 V
Pristine
0.0
1.0
2.0
3.0
4.0
R / Å
Li⁺
Li⁺
Li⁺
Li⁺

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-516**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Unraveling the importance of controlled architecture in multilayer electrode toward efficient electrocatalyst

구민수 김병수[1,*]

UNIST 에너지공학과 [1]UNIST 화학과

Even though traditional electrode fabrication methods such as simple mixing process have been used in various energy storage and conversion devices due to its handiness, however, these methods could not fully utilize and maximize the intrinsic properties of each active material. With the limited control over the internal structure of the electrode, it also often poses a significant challenge to elucidate the structure-property relationship between components within the electrode. Taking advantages of versatile layer-by-layer (LbL) assembly which can tailor nano-architecture of hybrid electrodes, here we report electrocatalytic thin films for methanol oxidation by adjusting the assembly sequence of LbL films based on the Au and Pd nanoparticles (NPs) and graphene oxide (GO) nanosheets. In case of co-assembled bimetallic LbL structure of (GO/Au/GO/Pd)n where respective Au and Pd NPs are supported with GO nanosheets, the electrocatalytic activity is significantly higher than that of respective monometallic LbL electrode (i.e. (GO/Au)n and (GO/Pd)n). To further investigate the architecture effect on the electrochemical behavior, Au and Pd NPs are assembled with GO in a different relative position of hybrid multilayer electrodes. It is proved that the electrocatalytic activity can be highly tunable by the position of metal NPs in the LbL structure, suggesting the structural dependence of charge and mass transfer between the electrolyte and the electrode, which is otherwise impossible to investigate in a simple conventional electrode fabrication method. Because of the highly tunable properties of LbL assembled electrodes coupled with electrocatalytic NPs, we anticipate that the general concept presented here will offer new insights in the nanoscale control over the architecture of the electrode toward development of novel electroactive catalysts.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-517**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly sensitive and simply operated electrochemical protease sensor toward point-of-care testing

박선화 양해식*

부산대학교 화학과

Protease sensors for point-of-care testing (POCT) require simple operation, a detection period of less than 20 minutes, and a detection limit of less than 1 ng/mL. However, it is difficult to meet these requirements with protease sensors that are based on proteolytic cleavage. This paper reports a highly reproducible protease sensor that allows the sensitive and simple electrochemical detection of the botulinum neurotoxin type E light chain (BoNT/E-LC), which is obtained using (i) low nonspecific adsorption, (ii) high signal-to-background ratio, and (iii) one-step solution treatment. The BoNT/E-LC detection is based on two-step proteolytic cleavage using BoNT/E-LC (endopeptidase) and L-leucine-aminopeptidase (LAP, exopeptidase). Indium-tin oxide (ITO) electrodes are modified partially with reduced graphene oxide (rGO) to increase their electrocatalytic activities. Avidin is then adsorbed on the electrodes to minimize the nonspecific adsorption of proteases. Low nonspecific adsorption allows highly reproducible sensor response. Electrochemical-chemical (EC) redox cycling involving p-aminophenol (AP) and dithiothreitol (DTT) is performed to obtain a high signal-to-background ratio. After adding C-terminally AP-labeled oligopeptide, DTT, and LAP simultaneously to a sample solution, no further treatment of the solution is necessary during detection. The detection limits of BoNT/E-LC in phosphate-buffered saline are 0.1 ng/mL for an incubation period of 15 min and 5 fg/mL for an incubation period of 4 h. The detection limit in commercial bottled water is 1 ng/mL for an incubation period of 15 min. The developed sensor is selective to BoNT/E-LC among four types of BoNTs tested. These results indicate that the protease sensor meets the requirements for POCT.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ELEC.P-518**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Halide Effects of Pt Nanoparticles on Their Electrocatalytic Performance in Oxygen Reduction Reaction

박현욱 박아현 권영욱*

성균관대학교 화학과

In the present work, we have synthesized Pt/C_KX (X = I and Br) samples in which 5 ~10 nm sized Pt Nanoparticles (NPs) on a carbon support by a single step ultrasound-assisted polyol synthesis (UPS) and studied the halide effects on Pt NPs of electrocatalytic performance for oxygen reduction reaction (ORR). In order to prepare Pt/C_KX (X = I and Br) samples, Pt(acac)2, KI (or KBr) and carbon support were dispersed in e ethylene glycol and irradiated by ultrasound for 3 h. Based on the structural characterization data, we found that Pt/C_KX samples have narrow size distribution and well-dispersed on carbon support. Electrocatalytic performance of samples was investigated by rotating disk electrode (RDE) measurement. Compared with commercial Pt/C, Pt/C_KX sample showed the enhanced ORR activity and durability in acid media. In conclusion, we demonstrated that the halide effects on Pt NPs can leads the enhanced electrocatalytic performance and durability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-519**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Insights into the Electrooxidation Mechanism of Formic acid on Pt layers on Au Examined by Electrochemical SERS

정화경 김종원*

충북대학교 화학과

The formic acid oxidation (FAO) on Pt has received great attention because of its technical importance in fuel cells. Recently, Pt layers modified on Au surfaces were reported to exhibit enhanced electrocatalytic activity for FAO reaction; however, the mechanistic details have not been clearly elucidated. In this work, the mechanism of FAO on Pt layers modified on Au surfaces using in situ electrochemical surface-enhanced Raman scattering (SERS) was investigated. The Pt layers with different the amount and coverage on dendritic Au rod (DAR) surfaces were fabricated using the self-terminating electrodeposition, wherein the amount of Pt were precisely controlled by applying a different number of potential steps (n) during the electrodeposition. The electrocatalytic activity of FAO was dependent on the Pt coverage and thickness on DAR@Pt(n), which was investigated by electrochemical SERS. The amount of CO produced by FA dehydration, the potential-dependent SERS intensity variation, and the Stark slopes were examined on different DAR@Pt(n) surfaces. The FAO behavior observed on DAR@Pt(1) surface could be supposed to proceed by a direct pathway. But, the SERS results presented in this work revealed that the indirect pathway involving CO as a reaction intermediate also occurred. However, the amount of CO produced by FA dehydration is relatively small compared to other DAR@Pt(n) surfaces. The potential-dependent SERS intensity and Stark slopes revealed that the adsorption strength between CO and Pt was quickly weakened during the positive potential excursion, which enabled the direct electrooxidation of FA. As the Pt coverage increased, a greater amount of CO was produced by FA dehydration, and the adsorbed CO persisted longer in the early stage of FAO. The direct electrooxidation of FA was mostly prohibited by the adsorbed CO initially produced by the dehydration of FA on DAR@Pt(n≥15). The present work provides insight into the mechanistic interpretation of FA electrooxidation on Pt-Au systems.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-520**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Rational Syntheses of Well-dispersed Pt-M (M=Fe, Co) core-shell Nanoparticles with Enhanced Electrocatalytic Performance in Oxygen Reduction Reaction

박아현 박현욱 권영욱*

성균관대학교 화학과

In this work, we have synthesized Pt-M/C (M = Fe and Co) samples in which 2 ~ 3 nm sized Pt-M nanoparticles (NPs) are formed on a carbon support by a one-step ultrasound-assisted polyol synthesis (UPS) and investigated their electrocatalytic performance for oxygen reduction reaction (ORR) in acid media. In order to prepare Pt-M/C samples, PtO2, Fe(acac)3 (or Co(acac)2) and carbon support were dispersed in ethylene glycol and irradiated by ultrasound for 3 h. Based on the structural analyses, Pt-M/C samples have well-dispersed core-shell NPs and narrow size distribution. Electrocatalytic performance of samples showed that Pt-M/C samples have improved ORR activity and durability than that of commercial Pt/C. Therefore, we demonstrated that Pt-M/C electrocatalysts have the advantage not only of reduced cost of materials but also of enhanced activity and durability.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-521**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An ultrasensitive and incubation-free electrochemical immunosensor using a gold-nanocatalyst label mediating outer-sphere-reaction-philic and inner-sphere-reaction-philic species

FangChiewSan 양해식*

부산대학교 화학과

It is not easy to simultaneously obtain both a fast redox reaction between two redox species in the presence of a nanocatalyst label (instead of an enzyme label) and vice versa, especially when the difference between their formal potentials is large. This communication reports a new nanocatalytic scheme based on the facts that the redox reaction between a highly outer-sphere-reaction-philic (OSR-philic) species and a highly inner-sphere-reaction-philic (ISR-philic) species is slow and that an OSR- and ISRphilic Au-nanocatalyst label can mediate the two different types of redox species. When the AuNC label is specifically bound to an indium–tin oxide (ITO) electrode, outer-sphere to inner-sphere electrochemical-nanocatalytic (ENc) redox cycling occurs in the sequence of OSR-philic ITO electrode, OSR-philic $Os(bpy)_2Cl_2^+/Os(bpy)_2Cl_2$, OSR- and ISR-philic AuNC, and ISR-philic hydrazine. ENc redox cycling allows high electrochemical signal amplification and thereby permits highly sensitive and incubation free detection of creatine kinase-MB. The calculated detection limit for the detection of creatine kinase-MB is approximately 20 fg mL^{-1}, indicating that the immunosensor is highly sensitive.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-522**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrogenerated chemiluminescence(ECL) ethanol biosensor based on Nafion/titania/ionic liquid composite film

양유나 이원용*

연세대학교 화학과

A highly sensitive biosensor for the detection of ethanol based on the $Ru(bpy)_3^{2+}$ ECL reaction with NADH has been developed. Ethanol is being produced and manufactured nowadays in a variety of different industries such as food and cosmetics. Due to the negative effects of ethanol use, such as obesity, stomach disorders, and even death, great attention for reliable determination methods for ethanol has been gained in the latest decades. For this reason, studies have been done in a variety of different fields in efforts to develop a sensitive and simple method for accurate determination of ethanol. Out of many different methods for the detection of ethanol, the $Ru(bpy)_3^{2+}$ electrogenerated chemiluminescence (ECL) method is one of the most selective and sensitive methods among them. In this study, the ECL ethanol biosensor was fabricated by casting a composite of ADH/$Ru(bpy)_3^{2+}$/ionic liquid/titania/Nafion onto the glassy carbon electrode. Ionic liquids, which are salts in liquid state, have unique chemical properties such as high electrical conductivity and good stability. The incorporation of ionic liquids into the composite film greatly improved the rate of electron transfer between $Ru(bpy)_3^{2+}$ and the electrode. As a result, the efficiency of $Ru(bpy)_3^{2+}$ ECL was greatly enhanced. The present biosensor showed improved ECL sensitivity as compared to the one without ionic liquids. The conditions related to the biosensor are optimized. Finally, the developed biosensor exhibited great performance for the determination of ethanol with high sensitivity, wide linear range, and good stability.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

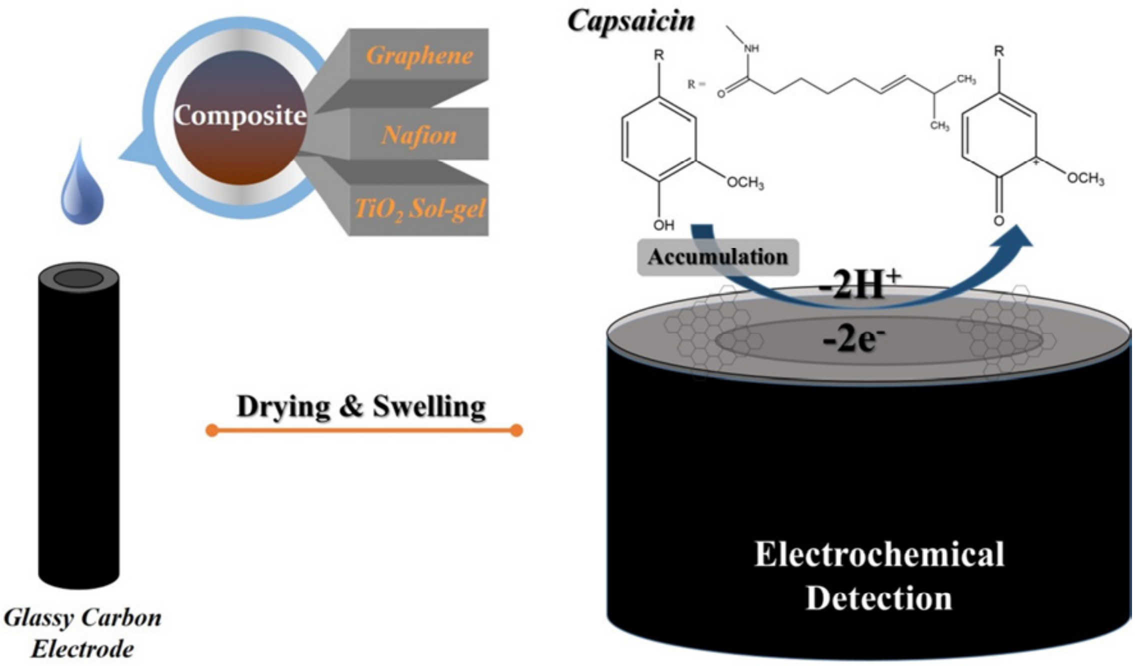
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-523**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly sensitive electrochemical capsaicin sensor based on graphene-titania-Nafion composite film

김동환 이원용*

연세대학교 화학과

A highly sensitive electrochemical capsaicin sensor utilizing graphene-doped sol-gel titania-Nafion composite film modified glassy carbon (GC) electrode is presented.Among a variety of different dishes around the world, hot and spicy foods are gaining popularity in recent years. Capsaicin is found in peppers in large amounts, and are known for their pungent taste. Not only is capsaicin the main reason for the pungent taste but also it is known for many health benefits such as high anti-tumoral property, anti-oxidation power, and protective effects against cholesterol and obesity. Thus, it has become more important to develop a simple and sensitive analytical method for the determination of capsaicin in food and pharmaceuticals.The graphene-titania-Nafion composite modified GCE facilitates the direct adsorption of capsaicin on the electrode surface via π-π interaction between capsaicin and graphene. Furthermore, the present composite modified electrode not only significantly enhances the oxidation peak current, but also decreases its oxidation peak potential, indicating that the graphene in the titania-Nafion composite clearly exhibits good electocatalytic ability to oxidize capsaicin. Under the optimized conditions, the present electrochemical sensor shows a linear response to capsaicin from 0.03 to 10.0 μM with a remarkably low detection limit of 8.6 nM (S/N = 3), which is much lower compared to those obtained with previously reported electrochemical sensors.Therefore, the present composite modified GCE can incorporate the advantages of each component, and hence becomes an ideal candidate as a sensitive electrochemical sensing platform for capsaicin. This work demonstrates an excellent analytical performance of the present composite-modified GCE in terms of sensitivity, linear dynamic range, reproducibility and stability, and it can be applied to the determination of capsaicin in real samples.


Composite
Graphene
Nafion
TiO2 Sol-gel
Glassy Carbon Electrode
Drying & Swelling
Capsaicin
R
NH
R =
O
CH3
CH3
OH
OCH3
R
+
OCH3
O
Accumulation
-2H+
-2e-
Electrochemical Detection

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-524**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Atomic Layer Electrodeposition of Pt on Nanoporous Gold Surfaces for Electroanalytical Applications

이은아 김종원*

충북대학교 화학과

백금은 전기화학적 촉매 활성이 뛰어난 금속으로 널리 알려져 있다. 하지만 매장량의 한계로 인한 높은 비용 때문에 사용의 제한이 따른다. 때문에 백금 양을 최소화 하기 위한 방법으로 얇은 백금 막 구조를 형성시키는 연구 결과들이 발표되었다. 기존에 발표된 간단한 펄스 기법인 원자 층 전착 (Atomic layer electrodeposition) 연구 결과에 따르면 평평한 금 기판 위에 -0.8 V 의 전위를 걸어주면 백금이 원자 수준으로 편평하게 한 층만 덮이고 석출된 백금 위에 수소 흡착이 일어나면서 더 이상의 석출이 일어나지 않는다. 본 연구에서는 선행 연구에서 사용했던 평평한 금 기판 대신 나노다공성 금 구조를 기판으로 활용하여 원자 층 전착법을 적용시키는 연구를 수행하였다. 전위와 시간에 따른 차이를 살펴본 결과 평평한 금과 달리 나노다공성 금 구조에서는 -0.8 V 의 전위를 걸어줄 때 시간에 비례하여 백금의 표면적이 점점 증가한다. 이 때의 백금 표면적 증가율은 나노다공성 금 구조의 표면적이 작을수록 더 빠른 시간 내에 일정해진다. 나노다공성 구조 위에 백금을 쌓을 때엔 일정한 전위를 계속 가해주는 것 보다 펄스 기법을 통해 전위를 가해주는 것이 더 효율적인 것을 확인하였으며, 한 펄스 당 환원 전위를 가해주는 시간이 10 초 일 때 백금 표면적 증가율이 가장 크고 드러나있는 금 표면적도 가장 작았다. 이러한 결과들을 바탕으로 나노다공성 금 표면 위에 백금을 효율적으로 덮을 수 있는 최적의 조건을 정하여 가해주는 펄스 수에 따른 백금 표면적 증가율에 대해 알아보았다. 덮인 백금의 표면적은 150 번의 펄스를 가해줄 때 나노다공성 금 구조의 표면적에 대해 최대 60 % 까지 증가하고 이때 덮이지 않은 채 남아있는 금은 4 % 정도로 나노다공성 금 구조가 대부분 백금으로 덮인 것을 확인할 수 있었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-525**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Spontaneous deposition of Au and Ir on porous Pt surfaces and their electrocatalytic behaviors

성문창 김종원*

충북대학교 화학과

전기화학적 석출 방법을 이용하여 간단하게 편평한 나노다공성 구조의 백금을 형성하였고, 이는 순수한 백금에 비해 넓은 표면적을 지니게 되어 전기화학적 촉매 활성에 우수한 특성을 지니고 있다. 본 연구에서는 이러한 편평한 나노 다공성 구조의 백금 위에 자발적인 반응으로 금 과 이리듐을 석출 시켜 두가지 금속의 특징이 섞여 있는 전극을 만들었다. 이를 이용하여 기존 편평한 나노다공성 백금 구조에 다른 금속을 석출 시키면서 큰 구조적 변화 없이 전기화학적 거동에 변화가 생김을 관찰 하였다. 선행 연구와 직접 실험을 통하여 금 과 이리듐의 자발적인 석출이 나노다공성 구조가 아닌 순수한 백금에서도 나타나는 것을 확인했다. 다만 나노다공성 구조의 백금에 금을 자발적으로 석출 시키는 경우와 순수한 백금에서 금을 자발적으로 석출 시킬 경우 차이가 존재하는데, 나노다공성 구조의 백금에서만 전극의 색이 뚜렷하게 금색으로 변화하였고, CV 에서 산화물 용해되는 봉우리의 이동이 보였다. 자발적으로 석출되는 과정에서 여러 변수들에 따라 차이를 관찰하였고, 이러한 두 가지 금속이 석출된 전극을 이용하여 포름산 산화 반응과 산소 발생 반응에 대한 활성을 살펴보았다. 포름산 산화 반응에 대한 활성은 금이 석출되는 시간을 적게 하였을 경우 미묘하게 증가하는 것이 관찰되었고, 금의 석출 양이 증가할수록 활성은 떨어졌다. 산소 발생 반응의 경우 금을 석출 시킬수록 활성이 감소하였다. 반면 이리듐을 석출 시킨 경우, 산소 발생 반응에 대한 활성이 더 좋아졌다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-526**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gas Ion Implanted Electrode Prepared by the SC-Electron Cyclotron Resonance Ion Source and Catalytic Effects

이동욱 윤장희[1] 심윤보*

부산대학교 화학과 [1]한국기초과학지원연구원 부산센터

The O^+ ion implanted glassy carbon electrode (GCE) using super conducting electron cyclotron resonance ion source (SC-ECRIS, 28 GHz) was characterized employing cyclic voltammetry, X-ray photoelectron spectroscopy, and Raman spectroscopy. The O^+ ion implanted electrode was effective on the oxidation of dopamine with blocking the negatively charged species. This has enabled the determination of dopamine in the presence of various interfering species, including ascorbic acid, in a phosphate buffer solution (pH 7.4). The implanted electrode revealed good performance for the detection of dopamine in a concentration range of 50.0 nM and 400.0 μM, with a detection limit (k = 3) of 10.0 ± 2.5 nM. The proposed electrode was employed for the determination of dopamine in a human urine sample and it was proven to be rapid, excellent selectivity, and stable amperometric responses.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-527**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cascading Alignment of Multilayered $SnO_2/WO_3/BiVO_4$ Inverse Opal Skeletons in Photoelectrochemical Water Splitting

윤건 강순형[1,*]

전남대학교 신화학소재공학과 [1]전남대학교 화학교육과

Tin dioxide (SnO2) inverse opals (IOs) having a pore size of approximately 260 nm in the 370 nm sized polystyrene bead (PS) templates were developed by a spin-coating-assisted sol−gel process. Upon this template, the SnO2/WO3 core-shell IOs were developed by the facile electrodeposition under a constant potential (−0.47 V vs. sat. Ag/AgCl), where the thickness of WO3 layer depended on the applied charge amount for WO3 electrodeposition (200−800 mC/cm2). As a control sample, a pure WO3 IO film with the same thickness of ~3.1 μm and a band gap (Eg) of 2.6 eV was also prepared in the same method. The pore diameter of the SnO2 IO structure declined noticeably as the charge amount of the deposited WO3 layer increased from 200 to 800 mC/cm2, leading to eventual coverage of the SnO2 IO structure in the WO3 (800 mC/cm2) layer. The optimum photoelectrochemical (PEC) response was achieved with the SnO2/WO3 (600 mC/cm2) IO electrode, which exhibited the highest photocurrent density (Jsc) of 2.8 mA/cm2 (0.5 VAg/AgCl) under full-sun conditions and 0.91 mA/cm2 (0.5 VAg/AgCl) under visible light, indicating that the enhancement of the Jsc under visible light contributed significantly to the improvement of the total Jsc, compared with the values for the pure SnO2, SnO2/WO3 (200, 400, and 800 mC/cm2), and WO3 IO electrodes. Furthermore, considering that the favorable cascading band alignment can boost the fast charge separation and transport through the conductive SnO2 IO skeleton, we try to develop the multilayered SnO2/WO3/BiVO4 IOs structure showing the well-matched band alignment. And then, the dual doped (W and Mo) BiVO4 layer was adapted in the surface layer due to the more narrowing Eg of ~ 2.4 eV. Herein, the PEC performance and other results would be presented.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-528**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Amperometric study of antibiotics transfer across liquid/liquid interfaces

김은미 이혜진*

경북대학교 화학과

본 포스터는 퀴놀론계 항생제를 검출하기 위해 서로 섞이지 않는 두 액체 사이에서 형성된 계면에서 항생제의 이동에 따라 달라지는 전류값을 측정한 결과를 나타내었다. 항생제가 존재하는 수용액 층의 pH 에 따라 유기층으로의 전이가 달라지게 되고, 이 현상에 기초하여 액체-젤 항생제 검출 센서 개발을 연구하였다. 순환전압전류법(Cyclic voltammetry)과 시차펄스벗김전위법(differential pulse stripping voltammetry)을 사용하여 얻은 전기화학적 결과를 얻었고, 이를 실제샘플에 적용한 결과를 나타내었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-529**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical conversion of CO2 into syngas using thiolate-protected Au25 and PtAu24 nanoparticles

임상혁 이용진 이동일*

연세대학교 화학과

The accumulation of carbon dioxide in the atmosphere is known for trigger to generate global warming. However, CO2 can be converted to starting material to make various chemicals and energy-rich carbon-containing fuels. The electrochemical conversion of CO2 is promising approach for handling CO2 accumulation. Unfortunately, the ectrochemical conversion of CO2 needs to meet high energy efficiency and reaction rates. So the discover and development of an efficient and robust electrochemical CO2 reduction catalyst are important challenges. In this poster, we demonstrate that the thiolate-protected Au25 and PtAu24 nanoparticles (Au25 and PtAu24 NPs) immobilized on carbon black/nafion (CB/Nf) coated onto glassy carbon electrode (GCE) can be utilized as electrocatalysts for CO2 conversion. Respective nanoparticles were synthesized and the composites were formed by sonicating with CB/Nf. The composites were cast onto GCE surface and electrolysis of CO2 was carried out in an H-Cell separated by nafion membrane at various applied potentials. Product analysis using gas chromatography indicated CO2 was efficiently converted to CO with high faradaic efficiency (>90%) at a moderate overpotential by using Au25 catalysts at neutral pH. Electrolysis using PtAu24 show the PtAu24 particles are more selective catalysts for H2 evolution reaction (HER) rather than CO2 reduction reaction (CO2RR). Finally, the origin of the vastly different selectivity observed for Au25 and PtAu24 particles is discussed.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-530**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical Study of Chemical Lift-off Lithography on Various Substrates

<u>김은성</u> 황성필* 박경순

고려대학교 신소재화학과

Chemical lift-off lithography (CLL) is one of soft lithography where small patterns on large substrate can be produced by removing of self-assembled monolayer (SAM) through covalent bond between activated stamp and SAM. In this study, CLL on Au and indium tin oxide (ITO) were investigated using electrochemical methods in terms of coverage, stability, and substrate-dependence. Alkanethiol and organic phosphonic acid are served as SAMs on Au and ITO, respectively. 11-Mercaptoundecanol (MUO) SAM on Au and hydroxyundecylphosphonic acid (HUPA) SAM on ITO were patterned by oxygen plasma-activated Polydimethylsiloxane (PDMS) stamp. Because siloxyl groups (Si-OH) of activated PDMS forms covalent bonds with terminal hydroxyl groups of SAM (-OH) on Au and ITO substrate, which enable detachment of SAM molecules from surface, called CLL. The interfacial properties of the SAM-modified electrodes and post-CLL electrodes were investigated by means of cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The results revealed that ca. 50 % of SAM on Au is shaved through CLL and remaining SAM is stable during subsequent SAM formation. For alkanephosphonic acid on ITO, similar behaviors were observed except smaller shaving ratio. Namely, only 12 % of SAM was removed in terms of electrochemistry but Lateral Force Microscope (LFM) images demonstrates that CLL also can be applied to the patterning of ITO.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-531**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Self-Assembled Flower-Like ZnO Microstructures as an Anode Material for Lithium-Ion Batteries

김한아 김종식*

동아대학교 화학과

Transition metal oxides have attracted significant attention as an alternative anode material for lithium-ion batteries because of their high theoretical capacity, stability, and environmental friendliness. Among them, zinc oxide (ZnO) has a higher theoretical capacity (987 $mAhg^{-1}$) than the commercial anode of graphite (372 $mAhg^{-1}$) through the alloy and conversion reactions with lithium ions. In addition, ZnO offers the advantages of low cost, non-toxic, and natural abundance. However, the severe capacity fading and poor cycling stability are caused by low electrical conductivity, slow diffusion of lithium-ion, and large volume change during charge/discharge processes of ZnO. In this work, N-doped carbon-coated ZnO microstructures (ZnO/NC) are synthesized through a facile hydrothermal reaction using urea and citric acid as nitrogen and carbon sources. The ZnO/NC has flower-like morphologies, which are composed of self-assembled primary nanoparticles, and exhibited a higher discharge capacity of about 876 $mAhg^{-1}$ after 50 cycles in the voltage range of 0.0-3.0 V at a rate of 0.1 C, compared to bare ZnO and carbon-coated ZnO (ZnO/C).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-532**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Improved ethanol oxidation in alkaline media using ultrafine PdmMn1-mOx binary catalysts on graphene

박동철 전승원*

전남대학교 화학과

Mixed-oxides binary alloyed catalysts (BACs) using a rare combination of graphene (G)-supported palladium (Pd) and manganese (Mn) have been synthesized with the addition of Pd and Mn metals in various ratios (G/$Pd_mMn_{1-m}O_x$) through a facile wet-chemical method. Thay have employed as an efficient anode catalyst for ethanol oxidation reaction (EOR) in alkaline fuel cells. The as-prepared G/PdmMn1-mOx BACs have been characterized by several instrumental techniques; the transmission electron microscopy images show that the ultrafine alloyed nanoparticles (NPs) are excellently dispersed onto the G. The Pd and Mn in G/$Pd_mMn_{1-m}O_x$ BACs have been alloyed homogeneously, and Mn appears in mixed-oxidized form in consequence of X-ray diffraction. The electrochemical performances including kinetics and stability of these catalysts toward EOR have been evaluated using cyclic voltammetry in 1 M KOH electrolyte. All G/$Pd_mMn_{1-m}O_x$ BACs have shown much superior mass activity and incredible stability than that of pure Pd catalysts (G/$Pd_1Mn_0O_x$, Pd/C and Pt/C). The well dispersion relating ultrafine size of NPs and higher degree of alloying are the key factor for enhanced and stable EOR electrocatalysis on G/$Pd_{0.5}Mn_{0.5}O_x$.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-533**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solar energy conversion by cyanobacterium *synechococcus sp.* through p-benzoquinone mediator

이진환 강나혜 김성현[1,*]

건국대학교 생명공학과 [1]건국대학교 특성화학부생명공학과

Photosynthesis is a highly developed system to harness enormous and inexhaustible solar energy, taking place in thylakoid membrane of plants, algae and cyanobacteria. Recently, the whole photosynthetic organisms or sub-cellular photosynthetic bio-components are being used as a converter of photo-bioelectrochemical devices to transduce solar energy to electrical energy. In this study, we have developed a method to convert solar energy into electric energy using cyanobacterium *synechococcus sp.* with a suitable mediator. We found that a suitable electron mediator is needed to acquire appreciable photocurrent. Among several possible mediators that transfer electrons between cyanobacteria and electrode, *p*-benzoquinone (PBQ) was found suitable. In order to improve the reversibility of PBQ on the electrode surface, we coated an indium tin oxide (ITO) electrode with reduced graphene oxide (RGO). Photocurrent highly depended upon the type and concentration of mediators, and stirring speed of the solution where dissolved PBQ molecules and cyanobacteria suspension exist. Maximum photocurrent of ca. 200 μA/cm^2 was observed at an applied voltage of 0.4 V vs. Ag/AgCl with 1 mM PBQ concentration under 1 sun irradiation. This result shows possibility of converting solar energy to electricity using photosynthetic microorganisms such as cyanobacteria and green algae.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-534**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Nitrogen-doped Carbon-coated Li_3VO_4 by In-situ Method as an Anode Materials for Lithium-Ion Batteries

박한솔 김종식*

동아대학교 화학과

Lithium-ion batteries (LIBs) have been utilized as effective power supplies for a wide range of applications such as laptops, mobile phones, and cameras owing to low cost, high capacity, and long life cycles. Nevertheless, it is necessary to explore the alternative anode material of graphite due to the increased demand of LIBs with large capacities in the fields of electric vehicles and hybrid electric vehicles. Because graphite has low theoretical capacity (372 mAhg-1). Lithium vanadate (Li_3VO_4) has been recently received attention a promising anode material for LIBs because of its high theoretical capacity of 394 mAhg-1, small volume changes, and fast diffusion rate of lithium ions during charge/discharge processes. However, the pristine Li_3VO_4 has a low initial coulombic efficiency because of its low electrical conductivity. In this study, nitrogen-doped carbon coated Li_3VO_4 (NC-LVO) was in-situ synthesized using dopamine (2-(3,4-dihydroxyphenyl)ethylamine). The NC-LVO exhibited the enhanced electrochemical performances in the voltage range of 0.0-3.0 V at a rate of 0.5 C compared to the pristine Li_3VO_4.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-535**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

수은 전기도금조에서의 수은의 전기화학적 회수 및 농도 모니터링

양대훈 윤수미 신운섭[1,*]

서강대학교 화학과 [1]서강대학교 화학과/융합의생명공학과

본 연구실에서는 이산화탄소를 포름산염으로 전환시키는 데에 치과용아말감을 적용하고 있는데, 전기도금법을 이용한 치과용 아말감 전극 제조시 발생하는 수은 도금 폐수를 최소화시키는 연구를 진행하였다. 사용된 수은도금용액을 Ar 분위기에서 -1.6 V (vs. Ag/AgCl)로 약 8~24 시간 동안의 전기분해를 하면 용액의 수은 농도가 수 ppb 이하로 감소되는 전기분해조를 구성하였고, Square wave anodic stripping voltammetry (SWASV)법을 이용하여 glassy carbon 전극으로 수은 농도 측정법을 확립하였다. 이를 통해 하수 배출 기준인 5 ppb 이하로 감소시켜 수은폐수 처리가 가능함을 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-536**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of Zinc Prussian blue analogue for transparent count electrode of electrochromic devices

정영희 곽준영[1] 김영일[2,*]

(주)애드크로 기술연구소 [1]애드크로 주식회사 대표이사 [2]부경대학교 화학과

Prussian blue(PB, iron(Ⅲ) hexacyanoferrate(Ⅱ)) is a well-known electrochromic material and its analogues with the Fe ions replaced by different combinations of transition metals show electrochromic characteristics. Zinc prussian blue analogue(Zn-PBA) which can be used transparent counter electrode due to the color change from clear to pale yellow at redox reaction. We synthesized Zn-PBA by simple co-precipitation and characterized by XRD, FE-TEM, SEM, UV-Vis spectrometer and Cyclic voltammetry. For roll-to-roll manufacturing, We used sol-gel technique, it is simplified method of preparing a uniform large-area film , and coated on ITO/PET.PB/Zn-PBA, V2O5/Zn-PBA, WO3/Zn-PBA and NiO/Zn-PBA devices were fabricated using this Zn-PBA film and adhesive gel-electrolyte. They showed excellent durability, high contrast ratio and short switching time.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-537**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

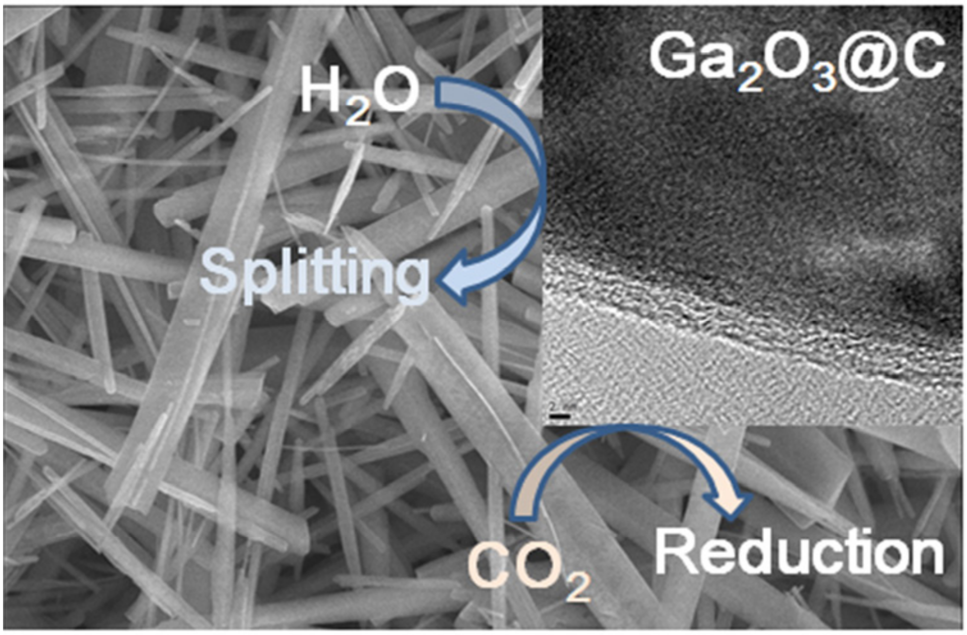
Photo-electrochemical Water Splitting and CO_2 Reduction over Ga_2O_3@C

윤희정 손영구[1,*]

영남대학교 이과대학/화학과 [1]영남대학교 화학과

Gallium oxide (Ga_2O_3) nanorods were prepared by a solvothermal method. Aerobic and anaerobic ethanol oxidation reactions were introduced to synthesize Ga_2O_3@C core-shell nanorods. Their physicochemical properties were examined by scanning electron microscopy, high resolution transmission electron microscopy, X-ray diffraction crystallography, X-ray photoelectron spectroscopy, Fourier Transform infrared spectroscopy, UV-visible absorption, and temperature-programmed reduction experiments. Photo-electrochemical water splitting and CO_2 reduction were examined to show that Ga_2O_3@C core-shell by aerobic ethanol oxidation reaction showed a dramatic enhancement in the performance.

Keywords: Ga_2O_3@C; CO_2 reduction; water splitting; photo-electrochemical reaction; anaerobic ethanol oxidation


Ga2O3@C
H2O
Splitting
CO2
Reduction

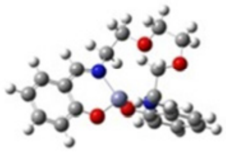
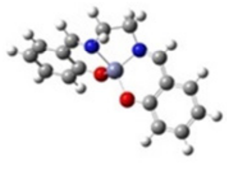
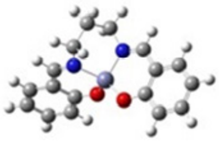
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-538**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fe_3O_4@SiO_2@Zn complexes for photo-electrochemical water splitting and CO_2 reduction

<u>남규석</u> 윤희정[1] 이지숙 강준길[2] 손영구*

영남대학교 화학과 [1]영남대학교 이과대학/화학과 [2]충남대학교 화학과

Photo-electrochemical water splitting and CO_2 reduction have recently attracted a considerable attention for energy and environmental issues. In the present research, we prepared lumino-magnetic core-shell structured Fe_3O_4@SiO_2Zn complex microspheres and examined water splitting and CO_2 reduction. Their physicochemical properties were examined by scanning electron microscopy, transmission electron microscopy, X-ray diffraction crystallography, Fourier transform infrared spectroscopy, photoluminescence, and magnetic measurement. We found that the core/shell structured zinc complex showed a dramatic enhancement in water splitting and CO_2 reduction.

ZnMD4	ZnENO	ZnPNO
		

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-539**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

One-Pot Electrodeposition of Cobalt and Silver for the Electrocatalysis of Oxygen Reduction Reaction

문신영 조윤빈[1] 이종목[1,*] 이영미[1,*]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학나노과학과

Since oxygen reduction reaction (ORR) is a sluggish reaction limiting the efficiency of fuel cells, there have been many studies about the ORR catalysts. Platinum (Pt) and its alloy materials are still the best catalysts. However, the limited amount and the high cost of Pt are the problem. Although silver (Ag) is one of the alternatives to Pt as an ORR catalyst through the direct four-electron transfer reaction in alkaline media, Ag still requires a high overpotential in the first step of ORR (O-O bond cleavage) due to the weak binding of the oxygen atom to Ag than Pt. To enhance its ORR catalytic effect, Ag is mixed with cobalt (Co) in this study. Cobalt helps the O-O bond breakage and then Ag reduces the resulting adsorbed atomic oxygen. In this work, Ag and Co are co-deposited on a glassy carbon rotating disk electrode (GC RDE) by one-pot deposition process using amperometry. Various bimetallic Ag and Co (Ag-Co) materials are deposited as a function of deposition charge and deposition time. The structure and electrocatalytic activities of Ag-Co are characterized by cyclic voltammetry (CV), linear sweep voltammetry (LSV), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The Ag-Co catalyst of which the metal precursor ratio of Ag:Co is 1:7 and the deposition time is 200 s (Ag_1Co_7-200) exhibits better catalytic activity than pure Ag and pure Co and the comparable activity to bare Pt disk electrode. 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 (2014R1A2A2A05003769).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-540**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Selectivity of Amperometric Nitric Oxide Sensor Controlled by Morphologies of Electrode Materials

김소희 하예진 이영미*

이화여자대학교 화학나노과학과

Nitric oxide (NO) plays various biological/physiological roles as an important gaseous signaling molecule in biological systems, such as neurotransmitter, modulator in both mammalian and non-mammalian species. As a detection tool, electrochemical methods have advantages of in situ and/or real time NO measurements. In the course of amperometric detection of NO in vivo, a variety of oxidizable biological interferents including anionic ascorbic acid, uric acid, neutral acetaminophen, as well as cationic dopamine can be measured at the same time. Recently, many researchers have tried to decrease the interruption from these interferents with various selective membranes such as chloroprene, PTFE (polytetrafluoroethylene), fluorinated xerogel and nafion. In this research, the selectivity to NO over common biological interferents is attempted to be obtained by controlling the platinum (Pt) electrode surface structure. Different morphologies of Pt are electroplated on a gold (Au) disk electrode (diameter = 2 mm) by varying the concentration of Pt precursor. The morphologies and compositions of the deposited Pt are characterized by field-emission scanning electron microscopy (FE-SEM). Also, the hydrophobicity of the electrode surface is confirmed by water contact angle with drops of deionized water on the electrode. The electrode amperometric responses to NO and interferents are tested at +0.75 V versus Ag/AgCl. The more hydrophobic structure shows the better sensitivity to NO over interferents. 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 (2014R1A2A2A05003769).

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ELEC.P-541**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of Amperometric/Potentiometric Dual Microsensor for Simultaneous Measurements of Carbon Monoxide and Potassium Ion

우주원 이영미*

이화여자대학교 화학나노과학과

Carbon monoxide (CO) and potassium ion (K+) are physiologically important species mediating vasodilation and neurotransmission. CO plays a role as a vasodilator through the activation of soluble guanylyl cyclase (sGC), generating guanosine 3’,5’-cyclic monophosphate (cGMP) which leads to K+ efflux. In addition, CO inhibits apoptosis triggered by K+ channel expression in neuron cells. To study the closely linked CO and K+ relations, a dual microsensor for simultaneous measurements of CO/K+ is developed. The sensor consists of a planar working electrode possessing platinum (Pt) and silver (Ag) microdisks (diameter of both disks = 76 µm). Both Pt and Ag microdisks are electrochemically etched to form recessed micropores. Pt micropore is filled with porous bimetallic layers via electrodeposition from metal precursor solutions in order. Finally, electrodeposited polymer and CO selective membrane are applied to obtain the selectivity to CO over common biological interfering species. Ag micropore is oxidized with FeCl3, silanized with trimethylchlorosilane (TMCS) and covered with K+ selective membrane consecutively. The sensitivity and selectivity of the dual sensor show the feasibility and suitability for the biological applications. 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 (2014R1A2A2A05003769).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-542**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical Properties of Highly Dispersive Gold Nanoparticles on Carbon Black

김여민 조아라 이영미* 이종목*

이화여자대학교 화학나노과학과

In this study, we synthesized highly dispersive gold nanoparticles on carbon black (HD-AuNPs/C) through a facile method in aqueous solution. Dispersity and size difference of Au NPs in carbon black were controlled by adjusting the concentration of reducing agent. The size and amount of Au NPs on carbon black were analyzed by scanning transmission electron microscopy (STEM), field emission scanning electron microscopy (FT-SEM), and energy dispersive X-ray spectroscopy (EDS). The mean diameters of AuNPs on carbon black in each sample varied from 2 to 6 nm. Electrocatalytic properties toward oxygen reduction reaction (ORR) were investigated at HD-AuNPs/Cs loaded electrodes with voltammetry. Among the samples, HD-AuNPs/C in which a mean diameter of AuNPs is 2.0 nm showed the best catalytic performance with the electron transfer number of 3.61 and the most positive half-wave potential which was even more positive than that of Pt/C.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-543**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Wood Charcoal Electrodes for Highly Stable Potassium and Sodium Ion Battery Anode

S.J. Richard Prabakar 표명호*

순천대학교 인쇄전자공학과

We for the first time report electrochemical K^+ and Na^+ intercalation/insertion in wood charcoal (WC) in a non-aqueous electrolyte, which can exhibit a reversible capacity of ~200 and 290 mAh.g^{-1}, respectively with excellent stability. Wood charcoal when treated at various temperatures from 600 to 1300^{o}C in an inert condition, showed a sequential transformation of the morphology and structure, much similar to the transformation from softcarbon to a pseudo-graphitic hardcarbon. Furthermore, the formation of new nanopores at high temperatures (at 1100^{o}C) in addition to the unique inherent capillary pores and cellular structure, significantly improve the porosity and thus the reversible insertion/intercalation of the alkali metal ions. The reversible flux of K^+ ions can be reasonably compared to the three staging intercalation process, as observed with graphite [1,2]. In contrast to the rapid capacity fading reported in the previous studies (~50 cycles) [1], the WC displayed excellent reversible stability for the intercalation of K^+ ions for more than 100 cycles at a current density of 0.02 A.g^{-1}. In a sodium ion battery, the WC delivered a reversible capacity of 290 mAh.g^{-1}, much likely to a non-graphitic carbon, but with a much superior cyclic stability and rate performance. The initial coulombic efficiency (CE) of potassium cell is ~55%, lower than ~75 % of Na cell, which promptly increases in the following cycles and eventually stabilizes at ~99.5%. The very high CE during the first few cycles in both cases reflects stabilization of a thinner SEI and a smaller irreversible capacity loss. The impressive rate performance of the WC may be attributed to the hollow structure with larger intergraphene spacing in turbostratic graphitic domains and the larger number of nanopores/nanovoids. We believe that this material derived from charcoal may open up a new paradigm toward rechargeable K/Na-ion batteries.References[1] Z. Jian, W. Luo, X. Ji, J. Am. Chem. Soc. 137 (2015) 11566−11569.[2] W. Luo, J. Wan, B. Ozdemir, W. Bao, Y. Chen, J. Dai, H. Lin, Y. Xu, F. Gu, V. Barone, L. Hu, Nano Lett. 15 (2015) 7671−7677.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-544**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Characterization and Catalytic Activity of Asymmetric Core-Shell Structured Au-Pd BimetallicNanoparticles Synthesized by the Galvanic Replacement Reaction

박성철 심준호* 안현준

대구대학교 화학과

Fuel cells are generally viewed as one of the most promising energy conversion systems in the next generation of sustainability. On the other hand, the high cost of fuel cells is one of the major challenges hindering its commercialization, because expensive Pt or Pt-based catalysts are currently used in these electrochemical devices to catalyze the cathodic oxygen reduction reaction (ORR). In this presentation, reduced graphene oxide (rGO)-supported asymmetric Au-core Pd-shell bimetallic nanoparticles (AuPd/rGO), i.e. Pd2+ is reduced only on the exposed Au(0) nanoparticle (GN) surface, were prepared using a simple two-step synthetic approach. First, negatively charged ~15-nm GNs were prepared and attached to the amine-functionalized positive surface of a glass slide. Second, the substrate of the adsorbed Au-core nanoparticles was added to the Pd precursor solutions (0.5, 5, and 10 mM of PdCl2, respectively), resulting in the deposition of a thin asymmetric Pd layer on the surface of the GNs via a tailored galvanic replacement reaction (GRR). The compositional/structural features were characterized by high-resolution transmission electron microscopy (HR-TEM), scanning TEM, X-ray diffraction (XRD), UV-Vis spectroscopy, and X-ray photoelectron spectroscopy (XPS). The catalytic activity of the AuPd/rGO was investigated by rotating disk electrode voltammetry in 0.1 M NaOH. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2014R1A1A2054826).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-545**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Synthesis of Carbon-supported Pd-core Pt-shell Nanoparticles and Their Enhanced Activity and Stability for Oxygen Reduction Reaction

Nguyen Thi Nguyet Anh 심준호*

대구대학교 화학과

In this presentation, we described a one-step method to synthesize Pd-core Pt-shell nanoparticles supported on carbon (Pd-Pt/C) through coreduction method without using any preformed seeds. A series of Pd-Pt/C with various Pd:Pt atomic ratios (%) were prepared with ascorbic acid as a reducing agent in the presence of nonionic surfactants. The main purpose of this work is to improve the catalytic activity with a lower Pt loading by combining Pt with other cheaper metal without loss of its performance and durability. The catalytic activity of the Pd-Pt/C for the oxygen reduction reaction (ORR) was investigated by rotating disk electrode voltammetry in acidic conditions. The Pd-core nanoparticles encapsulated by the porous Pt shells were confirmed by high-resolution transmission electron microscopy (HR-TEM), scanning TEM (STEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscope (XPS). This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2014R1A1A2054826).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-546**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Electrocatalytic Activity of Au-Ir Nanoparticles for the Oxygen Reduction Reaction

<u>안현준</u> 심준호*

대구대학교 화학과

Fuel cells have attracted great attention in recent years as a promising replacement for traditional energy system. Pt and its alloys as cathode catalysts for fuel cells are still the best electrocatalysts for oxygen reduction reaction (ORR), but the high cost and limited supply of Pt have been a major impediment to large-scale commercialization of fuel cells technologies. In this presentation, carbon-supported Au-Ir bimetallic nanoparticles (Au-Ir/C) were prepared using a simple two-step synthetic approach. First, gold nanoparticles were prepared and attached to the amine-functionalized positive surface of a glass slide. Second, the substrate of the adsorbed gold nanoparticles was added to the iridium precursor solution at various concentrations. The structures, morphologies and electrocatalytic activities of these nanomaterials are characterized by transmission electron microscope (TEM), scanning TEM, cyclic voltammetry (CV) and rotating disk electrode (RDE). This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2014R1A1A2054826).

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-547**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Simultaneous determination of trace heavy metal ions using iron oxide/graphene nanocomposite modified electrode

박원철* 김동원

서울대학교 융합과학기술대학원 융합과학부

Herein, we report a sensitive electrochemical sensor using iron oxide/graphene nanocomposite modified electrode in combination with in situ plated bismuth for the simultaneous determination of trace Zn^{2+}, Cd^{2+} and Pb^{2+} ions. The preparation of iron oxide/graphene nanocomposite was performed by a solventless thermal decomposition method. The synthesized nanocomposites were characterized by scanning electron microscopy, transmission electron microscopy, thermogravimetric analysis and X-ray diffraction. The electrochemical performance of the iron oxide/graphene nanocomposite modified electrode was also investigated. Differential pulse anodic stripping voltammetry was used for the electrochemical detection of Zn^{2+}, Cd^{2+}, and Pb^{2+} ions. Considerable parameters, such as the pretreating potential, applied bismuth concentration, pretreating time and pH of the supporting electrolyte solution were optimized for the simultaneous determination of trace heavy metal ions. The linear range of the modified electrode was measured to be 1-100gL^{-1} for Zn^{2+}, Cd^{2+} and Pb^{2+}. The limits of detection showed 0.11gL^{-1}, 0.08gL^{-1} and 0.07gL^{-1} for Zn^{2+}, Cd^{2+}, and Pb^{2+}, respectively. Repeatability (% RSD) was found to be 1.68% for Zn^{2+}, 0.92% for Cd^{2+} and 1.69% for Pb^{2+} using single sensor with 10 measurements. The potential for simultaneous detection of these heavy metal ions by the iron oxide/graphene nanocomposite modified electrodes was also demonstrated.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-548**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical characteristics and atomic-level simulation of reduced graphene oxide/manganese oxide composite film

유정준* 이찬우

한국에너지기술연구원 변환소재연구실

Supercapacitors have emerged as a new class of power sources. In this study, we fabricated an electrochemically characterized the reduced graphene oxide (RGO)/Birnessite (MnO2) composite film. The device shows superior volumetric capacitance, energy and power density. We also elucidate atomic scale operating mechanisms of RGO/MnO2 capacitor using state-of-the-art density functional theory calculations with RGO sheet/MnO2 nanoparticle models.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-549**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical areal performance of large scale thin film supercapacitors for flexible energy storage

유정준

한국에너지기술연구원 변환소재연구실

A thin film supercapacitor is one of the great alternatives of the rechargeable energy storage devices for the thin film electronics. Here, we have fabricated a thin film supercapacitor with the electrode dimension of 10 x 10 cm2 and the thickness of an entirely packaged device was ~300 u• m. The devices achieved moderate areal capacitance of ~10 mF/cm2 and showed good mechanical flexibility with no change in the capacitance of the device after 1000 bending cycles with the bending radius of 10 mm. They also showed superior long-term thermal stability for 2,000 hours under 60℃.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-550**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

In-situ Imaging for Li_2O_2 Decomposition during Charge of Li-O_2 Battery

홍미선 최희철[1,*] 변혜령[*]

KAIST 화학과 [1]POSTECH 화학과, 기초과학연구원 CALDES

Li_2O_2 decomposition process in a non-aqueous Li–O_2 battery has not been clarified yet due to lack of practical cell-analogue analysis system. We present in-situ imaging of Li–O_2 redox reaction on graphite electrode in ether-based electrolyte using electrochemical atomic force microscopy (ECAFM). During oxygen reduction at enough overpotential, thin film mainly composed of Li_2O_2 is deposited on the electrode with initial growth at edge planes of graphite. The film decomposes partially at low oxidation potential below ~3.7 V (vs. Li/Li^+) and fully at high oxidation potential over 4 V, which can represent complex current or potential profiles generally obtained during charging Li–O_2 battery. These observation indicates that the film has uneven local-reactivity for electrochemical oxidation, thereby requiring identification of local characteristics of Li_2O_2 and strategies to reduce oxidation overpotential in each potential range.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-551**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Volumetric capacitance of in-plane structure and out-of-plane structure for graphene based electrode

유정준[*] 이찬우

한국에너지기술연구원 변환소재연구실

It is a challengeable task to develop a supercapacitor that has a high volumetric performance as an ultra-small energy storage device. Even though nano carbon-based materials show very promising characteristics for this type of device, we need to find a new method if we want to develop a supercapacitor with a high volumetric capacitance. Here, we use a reduced multi-layer graphene oxide film as the electrode material, and fabricated planar type devices with in-plane structure and conventionally stacked devices with out-of-plane structure to compare their characteristics of volumetric capacitance. The Planar type devices with in-plane structure showed 2.5 times larger capacitance than the stacked type devices with out-of-plane structure, and also showed a larger energy density in the Ragone plot than the value reported for Lithium-ion thin film battery.

일시: 2016년 10월 12~14일(수~금) 3일간

장소: 부산 BEXCO

발표코드: **ELEC.P-552**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

전기삼투펌프를 적용한 체내 이식형 약물 주입기의 개발

손세미 신운섭[1,*]

서강대학교 화학과 [1]서강대학교 화학과/융합의생명공학과

체내 이식형 약물전달 펌프는 극심한 통증이 수반되는 암환자 및 만성통증환자에게 많이 사용되고 있다. 환자의 통증을 완화시킬 수 있는 척추의 최적 위치에 카테터를 통해 0.5 ~ 4 mL/day 속도로 척수강에 모르핀을 지속적으로 주입함으로써 통증을 완화시킨다. 척수강 내에 약물을 직접 투여하는 것은 경구 투여량의 1/300, 정맥 투여량의 1/100 과 동일한 효과를 나타내며, 다른 부위로 약물이 순환되지 않기 때문에 부작용이 적고, 체내 이식형이므로 운동이나 샤워 등 환자의 일상 생활에 불편을 주지 않는 장점이 있다. 현재 이러한 펌프는 전량 고가로 수입되어 활용되고 있어 통증환자들이 활용하기에 경제적으로 부담이 되고 있다. 본 연구실에서 개발된 전기삼투펌프는 초소형, 초경량이며 저전력 구동이 가능하고, 최근 오랜 기간 안정되게 작동될 수 있는 방법을 개발하였기 때문에 이를 대체하기 위한 펌프로 개발 가능했다. µL 단위의 유량 컨트롤, 초저전력 구동 등을 구현하여 전기삼투펌프가 체내 이식형 약물전달 펌프로서 적합함을 확인하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-553**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

전기삼투펌프를 이용한 세포간액의 추출

김석준 이상섭 신운섭[1,*]

서강대학교 화학과 [1]서강대학교 화학과/융합의생명공학과

Ultrafiltration technique 을 통해 세포간액을 추출하려는 시도는 기존부터 있어왔다.[1] Microdialysis techniques 또한 당농도를 측정하거나 neurotransmitter 등으로 응용하기 위한 연구가 많이 진행되어 이미 상품화가 된 사례도 있다.[2,3] 이러한 기술들은 microdialysis fiber 를 수술을 통해 체내로 삽입하게 되며 초소형 펌프를 사용하여 유체를 컨트롤하는 형태로 되어있다. 본 그룹에서는 전기삼투 펌프와 여러 가지 종류의 프로브를 사용하여 지속적으로 매우 느린 유속을 유지하며 세포간액을 추출하는 기술을 개발하였으며 이를 patch type 의 연속혈당측정 시스템에 응용하고자 하였다.

[1] G. L.-Vogt, E. Janle, S. R. Ashc, K. Venemaa, J. Korf "Utilization of in Vivo Ultrafiltration in Biomedical Research and Clinical Applications" Life Sci 2003, 73, 2005-2018[2] P. Nandi, S. M. Lunte "Recent Trends in Microdialysis Sampling Integrated with Conventional and Microanalytical Systems for Monitoring Biological Events: A Review" Analytica Chimica Acta 2009, 651, 1-14[3] J. Korf, K. D. Huininka, G. A. Posthuma-Trumpie "Ultraslow Microdialysis and Microfiltration for In-line, on-line and off-line Monitoring" Trends Biotechnol 2010, 28, 150-158.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-554**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical Grafting of Carbon Nanotubes with Dedrimer-Encapsulated Nanoparticles: Toward the Facile Platforms for Electrical/Electrochemical Biosensor

이창석 김동욱 홍수정 김태현*

순천향대학교 화학과

We present a facile and efficient electrochemical method for the fabrication of a carbon nanotube–dendrimer hybrid material. The material has been prepared by cyclic voltammetry of carbon nanotubes (CNTs) on solid substrate in an electrolyte containing amine-terminated sixth-generation polyamidoamine dendrimers. Single-walled carbon nanotubes (swCNTs), decorated with dendrimer molecules, have been generated on polyethylene terephthalate (PET) film during the electrolysis with no further chemical treatment. Pre-synthesized nanoparticles in the form of dendrimer-encapsulated nanoparticles (DENs) have also been assembled onto swCNTs via electrochemical grafting method. Cyclic voltammetry, contact angle measurement and confocal laser scanning microscopic characterization reveal the formation of swCNT-dendrimer hybrid structure by covalent interaction. We also demonstrated feasibility of the resulting DEN-swCNTcomposites as electroanalytical sensing platforms in voltammetric and field-effect transistor (FET)sensors using the enhanced electrocatalytic redox activity of the Pt DEN-swCNT composites on PET film.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-555**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

이산화탄소의 옥살산염으로의 전기화학적 전환

김지나 신운섭[1,*]

서강대학교 화학과 [1]서강대학교 화학과/융합의생명공학과

본 연구실에서는 치과용아말감전극을 활용하여 이산화탄소의 유용한 화합물로의 전환을 진행하고 있다. 기존에 납전극과 acetonitrile 용매를 활용하여 이산화탄소를 옥살산염으로 전환시킨 예가 있는데[1], 치과용 아말감 전극을 활용하여 비교 연구를 진행하였다. 용매로 Dimethyl Sulfoxide 를 사용하여 용매의 휘발성이 없는 상태에서 전기분해를 진행할 수 있었고, 전류 효율도 기존 89%에서 100%로 증가시킬 수 있었다. 침전물 형성을 위한 산화전극으로 Zn, Mg, Al 을 비교해 본 결과, Zn 가 가장 우수한 성능을 보여주었다.[1]Lixu Lei et al (2013) J Solid State Electrochem 17:2789–2794

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-556**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemcal preparation of CIGS thin films

김은혜 연유범[1] 정찬용[2] 이치우[3,*]

고려대학교 세종캠퍼스 소재화학과 [1]고려대학교 과기대 소재화학화 [2]고려대학교 소재화학과 [3]고려대학교 신소재화학과

The chalcopyrite $CuIn_xGa_{(1-x)}Se_2$ (CIGS) is the most effective light-absorbing materials for thin film photovoltaic solar cells. We wish to report the electrodeposition of CIGS thin films in ambient laboratory conditions, and to suggest the electrochemical conditions to prepare stoichiometric CIGS thin films of Cu/(In + Ga) = 0.9. In acidic solutions containing Cu^{2+}, In^{3+}, Ga^{3+} and Se^{4+} ions, the CIGS films of different Cu/In/Ga/Se chemical compositions were electrodeposited onto onto different electrodes by means of chronoamperometry, chronopotentiometry, rotating disk voltammetry and electrochemical quartz crystal microbalance method. The structure, morphology and chemical composition of electrodeposited CIGS films were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), and Energy dispersive X-ray spectroscopy (EDS), respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-557**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Syntheses, characterization, and electrochemical properties of Cu_2SnS_3 nanoparticles and Cu_2SnS_3/reduced graphene oxide composite for Li-ion batteries

황차환 옥강민*

중앙대학교 화학과

Ternary Cu_2SnS_3 (CTS) have been studied as a solar absorber material owing to their p-type semiconducting property, appropriate band gap energy (~ 1.2 eV), and high absorption coefficient (~10^5 cm^{-1}). Recently, these sulfide-based chalcogenide materials have been also used in Li-ion battery anode. In the discharge process, CTS reductive decompose to Cu metal, Sn metal, and Li_2S. Then Sn metal can further store the Li ion to Li_xSn such as silicon metal alloy anode, so the CTS exhibit high theoretical capcity (815 mAh g^{-1}). However, reductive decomposition and volume expansion of CTS at the lithium storage process cause the loss of electric current path, which structural degradation results in the low coulombic efficiency and capacity fade. In this research, CTS nanoparticles and CTS/reduced graphene oxide (rGO) composite were synthesized through a simple sonochemical method to overcome the structural failure in the charge/discharge process. The high power sonochemical reaction is able to induce an effective surface attachment on the template materials homogenously in a short reaction time. The prepared CTS/rGO composites were calcined at various temperatures to crystallization. The first cycle discharge capacity of calcined CTS/rGO composite was about 1000 mAh g^{-1} in the voltage range of 2.5~0 V at the current density of 100 mAh g^{-1}.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-558**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

N, F co-doped activated carbon for supercapacitors at high temperature condition

김주연 노광철[1,*]

한국세라믹기술원 에너지소재센터 [1]한국세라믹기술원 에너지효율소재팀

Recently, electrochemical double layer capacitors (EDLCs) have been extensively developed to satisfy and high-temperature the increasing demand in the hybrid power sources for electrical vehicles (EV) and other energy fields. Activated carbon (AC) for the electrode materials of EDLC has been widely researched because of its high specific surface area and low costs. The major disadvantages of oxygen-containing function groups of AC, especially high temperature, are quite susceptible to electrolytes because of generating of gas. Nitrogen and fluorine co-doped activated carbon (NF-AC) exhibits significantly improved electrochemical capacitive performance with kinetic enhancement compared to raw activated carbon at high temperature (85°C). This indicated that NF-AC tends to form the electric double-layer ions on its surface rapidly as a result of the increase electrical conductivity attributed to the decrease of oxygen-containing function groups. The electrochemical improvement of NF-AC proves that N, F co-doping is a very effective method for providing greater possibilities for supercapacitor applications in high temperature.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-559**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A metal-free bifunctional electrocatalyst for oxygen reduction and oxygen evolution reactions in alkaline media

이치호 이상욱[1,*]

한양대학교 바이오나노공학과 [1]한양대학교 응용화학과

In the recent years, water splitting has attracted substantial interest including key processes oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) in renewable energy conversion and storage devices such as the cathode of fuel cells, metal-air batteries and supercapacity. Here we designed C3N4 structures doped with heteroatoms, P, S or PS, as outstanding electrocatalysts for following key reactions by performing density functional theory (DFT) calculation in both alkaline and acidic environment. The results show that the substitution of nitrogen or carbon at C3N4 by P and S results in the best performance in terms of volcano plot between the activity of OER and ORR reactions and the adsorption free energy of intermediates on doped C3N4 materials. For P,S-doped C3N4, the lowest OER and ORR overpotentials were estimated to be 0.46 V and 0.36 V in alkaline media and 0.55 V and 0.37 V in acidic media, which are comparable to state-of-the-art RuO2 and Pt catalyst, respectively. OER and ORR with the minimum overpotentials arises from different nitrogen and carbon sites of the same structure in alkaline and acidic environment, respectively. These calculations suggest that substitution of P and S on C3N4 can increase the catalytic activity of OER and ORR reactions as efficient electrocatalysts for key energy conversion processes including oxygen evolution reactions and oxygen reduction reactions.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-560**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical properties of MnO_2/MWCNT composite in neutral aqueous electrolytes for supercapacitors

채지수 노광철[1,*]

한국세라믹기술원/성균관대학교 에너지소재팀/에너지과학과 [1]한국세라믹기술원 에너지효율소재팀

Manganese dioxide (MnO_2)/multi-walled carbon nanotubes (MWCNTs) nanocomposites have been prepared as electrode materials for supercapacitor applications. The materials were synthesized using by simple immersion of the MWCNTs into a $KMnO_4$ aqueous solution. The morphology and microstructure of samples are examined by scanning electron microscopy (SEM), transition electron microscopy (TEM), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). Electrochemical properties are characterized by cyclic voltammetry (CV) and galvanostatic charge/discharge. Results show that a nanosized MnO_2 uniform layer covered the surface of the MWCNT and the original structure of the pristine MWCNT was retained during the coating process. The cyclic voltammetry curves demonstrate that the specific capacitance of the composite electrode reaches 224 and 109 F g^{-1} at 1 and 200 mV s^{-1}, respectively, which is significantly higher than that of a pure MWCNT electrode.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-561**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical performance of nitrogen-doped activated carbon by urea for supercapacitors

강원섭 장수진[1] 노광철[2,*]

한국세라믹기술원 에너지소재센터 [1]한국세라믹기술원 에너지소재/신소재공학 [2]한국세라믹기술원 에너지효율소재팀

In this study, we propose a simple approach for the synthesis of nitrogen-doped activated carbon (N-doped AC) via thermal annealing with urea, to improve the cycle stability and rate capability of electric double layer capacitor (EDLC) by minimizing the oxygen functional group of AC. And we compared the effect of urea by concentration. In order to confirm chemical structure and composition of the materials, XPS and Raman analysis were conducted. The pore structures were characterized by N2 adsorption/desorption isotherm at 77 K using the BET equation and BJH method. The electrochemical properties of N-doped ACs were accumulated by cyclic voltammetry, impedance spectra, and charge–discharge cycling performance in non-aqueous electrolyte. As a result, Electrochemical measurements indicated that N-doped AC exhibits enhanced rate capability and cycle performance as compared with pristine AC.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-562**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

One-pot preparation of nickel-nickel oxide nanoparticles for enzyme-free glucose sensing with higher sensitivity in alkaline media

BEGUM HALIMA 전승원*

전남대학교 화학과

The Nickel-nickel oxide nanoparticles (NiNiONPs) was directly electrodeposited onto glassy carbon electrode (GCE) by electrochemical deposition method using cyclic voltammetry (CV) technique in acid solution and have been used as a highly sensitive enzyme-free glucose sensor in alkaline media. The characterizations of the sensor probe reveal that Ni forms as a homogeneous nanoparticle structure during deposition and afterwards NiO-shell form onto the Ni-core. The electrochemical deposition conditions of the Ni-core were verified and 20 cycles at 50 mV s^{-1} was the optimized. Electrochemical activity of the modified electrode towards the oxidation of glucose was studied using various electrochemical methods and it showed long linear range (2 • M to 13 mM) with higher sensitivity (1189.8 • A mM^{-1} cm^{-2}). Moreover, the proposed method was successfully applied to determine glucose in real sample with satisfactory results.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-563**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

High sensitive glucose sensor using Chitosan-Multiwalled Carbon Nanotubes Composite

이보희 이창준 최영봉 김혁한*

단국대학교 화학과

Direct electrochemistry of a glucose sensing was studied with glucose oxidase(GOx)-multiwalled carbon nanotubes (MWCNTs)-chitosan composite. Chi-MWCNTs (1 mg/mL) of 50 μL was loaded onto indium-tin oxide (ITO) electrode, and then dried overnight. glucose oxidase (GOx, 20 mg/mL) of 20 μL was casted onto the prepared Chi-MWCNTs ITO electrode, and then dried at room temperature for 3days without cross-linker or binder. GOx/Chi-MWCNTs/ITO was rinsed with distilled water (DW) after GOx completely dried for remove the unbinding substrate.Characterizations of the prepared electrodes were investigated by scanning electron microscope (SEM) and fourier transform infrared spectroscopy (FT-IR).The result electrical signals were measured by cyclic voltammetry (CV).We confirmed no effect of interference such as ascorbic acid (AA) and uric acid (UA) onto the GOx/Chi-MWCNTs/ITO electrode.The superior performance of the biosensor is attributed to high conductivity of MWCNTs, and good biocompatibility of chitosan, and optimized chitosan-CNT ratio.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-564**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optimization of hydrophilic polymers for covering of multi walled carbon nanotubes in directly determination of glucose

조호진 전수연 최영봉 김혁한*

단국대학교 화학과

A hydrophilic polymers were optimized involving multi walled carbon nanotubes (MWCNTs). MWCNTs were covered with hydrophilic polymers such as poly(acrylic acid)-poly(vinyl imidazole) (PAAc-PVI), poly(acrylic acid)-poly(vinyl pyridine) (PAAc-PVP), poly(acrylic amide)-poly(vinyl imidazole) (PAAm-PVI), and poly(acrylic amide)-poly(vinyl pyridine) (PAAm-PVP) under ethylene glycol (EG) with ultra-sonicate, and then purified using centrifuge and filtration. Glucose oxidase (GOx) was dropped hydrophilic polymer/MWCNTs absorbed indium tin oxide (ITO) electrode, and then GOx/hydrophilic polymer/MWCNTs/ITO were dried after rinsing using distilled water (DW). The surface morphology of the hydrophilic polymer/MWCNTs casted onto ITO electrode were examined by scanning electron microscopy (SEM). To analyze thermal characteristic, that were examined by thermogravimetric analyzer (TGA) and dispersion force of that were examined by measuring zeta potential analyzer. The electrical signals for determination of glucose were measured by cyclic voltammetry (CV) and amperometry. And the result shown that quantification with linearly calibration curve under the various concentrations of glucose. Also, our electrodes were showed no interferences from common physiologic interferences such as ascorbic acid (AA) or uric acid (UA). Therefore, this approach allowed the development of a simple, high sensitivity, and disposable electrochemical glucose biosensor.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-565**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Silver and cobalt oxide alloyed nanoparticles onto graphene for better electrocatalytic oxygen reduction reaction

주유리 전승원[*]

전남대학교 화학과

The electrochemically reduced graphene oxide-based silver and cobalt alloyed nanoparticles (NPs) has been synthesized by an electrochemical method (denoted as AgCo/ERGO) for comparatively better oxygen reduction reaction (ORR) in alkaline media. The successful alloyed formation and subsequent electrochemical reduction in the process of catalyst preparation have been confirmed using X-ray photoelectron spectroscopy. The XPS shows electrochemical reduction has been done successfully with the increasing of C/O ratio. The morphological analysis shows the AgCo alloyed NPs are well set on to the ERGO with better dispersion. Also, the X-ray diffraction (XRD) data reveals that the Co is presents with the oxidized form into AgCo alloyed NPs. The electrocatalytic activities have been verified using cyclic voltammetry (CV) and hydrodynamic voltammetry techniques in 0.1 M KOH electrolyte. The as-prepared AgCo/ERGO catalyst has been proven an efficient non-novel-metal electrocatalyst with better electrocatalytic activity, stability, and tolerance to crossover effect than other catalysts including Pt/C for ORR due to higher degree of alloy formation and better dispersion of AgCo NPs into ERGO.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-566**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

2,3-diaminopyridine functionalized graphene supported palladium nanodendrites for improved electrocatalytic oxygen reduction reaction in alkaline fuel cell

<u>YASMIN SABINA</u> 전승원*

전남대학교 화학과

The electrochemical deposition of Pd nanodendrites on 2,3 diamino pyridine functionalized graphene oxide (2,3DAP-GO/Pd) has been investigated for the oxygen reduction reaction (ORR) in alkaline solutions. The as prepared material 2,3 DAP-GO/Pd has been characterized by various instrumental methods. The morphological analysis shows the unique naodedrites like Pd are dispersed onto the 2,3 diamino pyridine functionalized graphene oxide (2,3DAP-GO) with better dispersion. The electrocatalytic activities have been verified using cyclic voltammetry (CV) and hydrodynamic voltammetry techniques in 0.1 M KOH electrolyte. The resultant 2,3DAP-GO/Pd shows higher catalytic activity toward ORR with more positive onset potential and higher cathodic current density. It is also noteworthy that the 2,3 DAP-GO/Pd exhibits a four-electron transfer pathway for ORR with lowering H_2O_2 yield. The determined Tafel slope and the chronoamperometry stability of 2,3 DAP-GO/Pd nanodendirtes electrocatalysts were comparable to the counterpart Pt nanoparticles supported on carbon.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-567**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of mesoporous carbon electrode on discharge product morphology and recharge potential in a Li-O_2 battery

Arghya Dutta 변혜령*

KAIST 화학과

A non-aqueous Li-O_2 battery is thought to be one of the most promising energy storage technologies because of very high theoretical specific energy of ~3500 Wh/kg. However, realization of this battery is hindered by high recharging overpotential, which is responsible for low stability of both non-aqueous electrolyte and carbon electrode, leading to serious side reactions. The fundamental reason behind the high overpotential is believed to be very poor conductivity of solid Li_2O_2 as a discharge product, which requires further energy to be electrochemically decomposed (Li_2O_2 ---> $2Li^+ + O_2 + 2e^-$). Interestingly, the conductivity of Li_2O_2 has direct relation with its crystallinity and morphology that in turn affect the recharge potential. The amorphous Li_2O_2 has been found to have much higher ionic and electronic conductivities compared to the crystalline Li_2O_2.[1] Additionally, small size of Li_2O_2 with large contact area to the carbon electrode can aid in its smooth decomposition at low charging potential.[2] Here we present a catalyst free mesoporous carbon (CMK-3) cathode promoting the formation of amorphous and flake-shaped Li_2O_2 which greatly lowers the recharge potential. We propose that the surface structure of mesoporous carbon electrode is the key to implant the Li_2O_2 flakes during discharge. We further show that not only amorphous nature of Li_2O_2, but additionally shape of the deposited Li_2O_2 also plays vital role in reducing the recharge potential.The discharge/charge potential profiles of CMK-3 and other carbons such as LPC-80 (a macroporous carbon with average pore diameter of 80 nm), ketjen black (KB) carbon particle and multi-walled carbon nanotube (MWCNT) are compared with a limited discharge capacity using 0.5 M LiTFSI in TEGDME. Two well-known oxygen evolution reaction (OER) catalysts Ru and Co_3O_4 nanoparticles loaded on MWCNT electrode are also included for comparison. Strikingly, the CMK-3 based Li-O_2 cell shows a very low recharge potential below 3.5 V until ~75% of recharge process. The pivotal reason for the decreased overpotential may be associated with an amorphous and flake-shaped Li_2O_2 vertically formed on the surface of CMK-3 during discharge, which are almost completely decomposed at the low recharge potential. Morphological analysis and online electrochemical mass spectroscopic (OEMS) studies indeed show that the Li_2O_2 flakes are decomposed at potential well below 3.5 V. This result is quite different from other carbon electrodes such as ketjen black (KB) carbon particle, multi-walled carbon nanotube (MWCNT) and LPC-80 consisting of spherical pores with a diameter of ~80 nm, where higher recharge potentials shown can be correlated with typical structure of thick Li_2O_2 film deposited on the carbon surface. This reveals that the surface structure of the carbon electrode is key to implant the Li_2O_2 morphology. In addition, the CMK-3 carbon with mesoporous structure associated with some micropores and surface defects promotes the formation of Li_2O_2 flakes. A detailed morphological and electrochemical analysis will be discussed in the presentation.References:1)Tian, F.; Radin, M. D.; Siegel, D. J., *Chem. Mater.*, 2014, *26*, 2952-2959.2) Dunst, A.; Epp, V.; Hanzu, I.; Freunberger, S.; Wilkening, M., *Energy Environ. Sci.*, 2014, *7*, 2739-2752.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-568**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ionic liquid-derived graphitic actviated carbon for ultracapacitors

김목화 임건해 노광철[1,*]

한국세라믹기술원 에너지소재센터 [1]한국세라믹기술원 에너지효율소재팀

The use of an ionic liquid as a precursor for producing activated carbon offers a number of known benefits, not least of which is the fact that introduces nitrogen atoms into the final structure. Using this knowledge, we have demonstrated that the chemical activation of carbon derived from an ionic liquid (EMIM-dca) creates a structure that combines the high surface area of micro/mesopores with the excellent electrical conductivity of a graphitic structure due to the removal of nitrogen. These properties are attributed to the removal of nitrogen, which causes a rearrangement of atoms to create a new structure. To evaluate the potential of ionic liquid derived activated carbon (IL-AC) for use as an electrode material, it was used to assemble a two-electrode system for a supercapacitor. The rate performance was assessed through plots of specific capacitance versus current density for devices based on either IL-AC or commercial activated carbon. Note that despite this decrease in specific capacitance with increasing current density, 92% of the capacitance at 1.0 mA cm-2 is still retained at 30 mA cm-2; a result which shows a consistently higher specific capacitance at increased current density than commercial activated carbon. As this material could be applied in other high-power energy storage systems, we believe that the findings of this study are relevant to the scope of your journal and will be of interest to its readership.

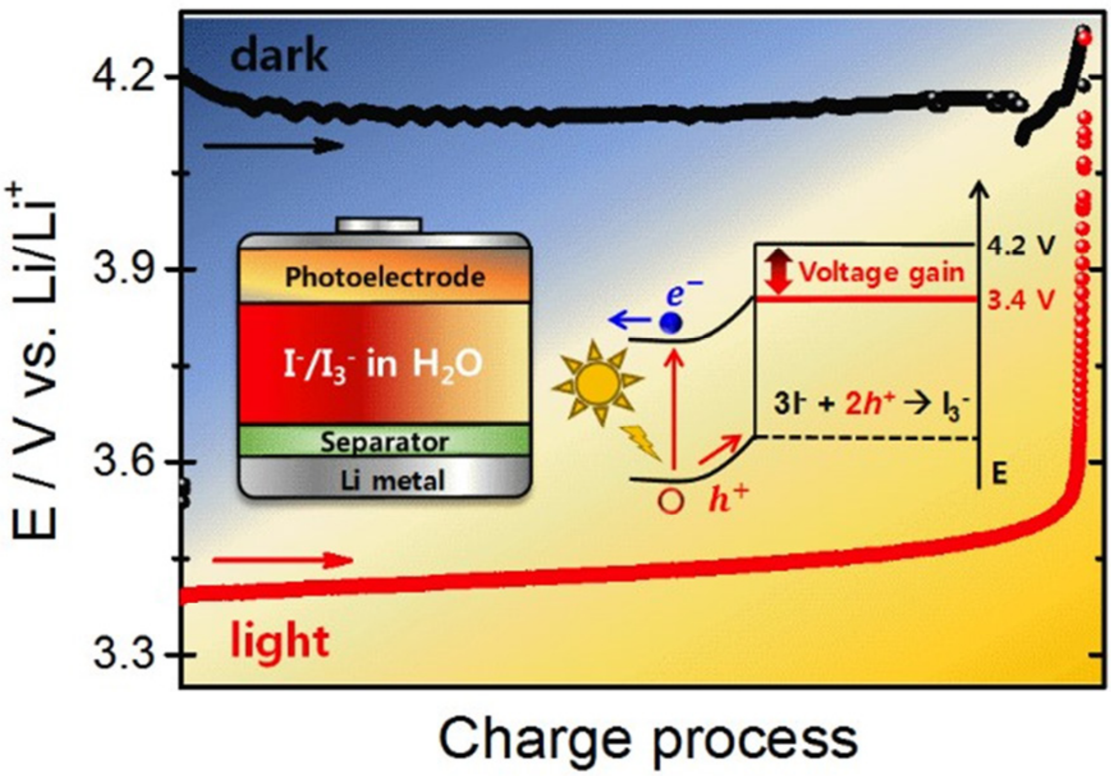
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-569**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

High Energy Efficiency and Stability for Photo-Stimulated Aqueous Lithium-Iodine Batteries

GEORGIOS NIKIFORIDIS **변혜령**[*]

KAIST 화학과

We demonstrated photo-stimulated lithium-iodine (Li–I2) redox cells integrated with a hematite photo-cathode, applicable on energy storage systems (ESSs). The hematite photo-electrode possesses low cost, visible light region of light absorption and inertness to aqueous electrolytes, which allows for stable production of photocurrent under illumination. In the aqueous Li–I2 redox cells, the harnessing photo-energy generates photo-carriers that promote I¬– oxidation process without electrolysis of the aqueous solution and in situ store electricity (Fig. 1). The photo-stimulated charge process improves voltaic (99.2 %) and energy efficiencies (85%) of the Li–I2 redox cells for a total of 30 deep charge-discharge cycles. The hematite is profoundly stable in aqueous I–/I3– catholyte and demonstrates over 600 h cycling without noticeable performance decay and photo-corrosion. This achievement accentuates photo-induced ESSs with ameliorating energy efficiency in the condition of amenable maintenance.


dark
light
4.2
3.9
3.6
3.3
E / V vs. Li/Li$^+$
Charge process
Photoelectrode
I$^-$/I$_3^-$ in H$_2$O
Separator
Li metal
e^-
h^+
Voltage gain
4.2 V
3.4 V
3I$^-$ + 2h^+ → I$_3^-$
E

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-570**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced electro-conductivity of metal substituted β-LiV1-xMxOPO4 cathode materials for lithium-ion batteries

박다정 류광선*

울산대학교 화학과

Lithium vanadyl phosphate (LiVOPO4) is an attractive cathode for lithium ion batteries with a high operating voltage 4.0V in phosphate poly-anion cathode materials and good theoretical capacity of 166mAh/g. However, the main defects such as poor electrical conductivity and low lithium ionic conductivity are drawback for its application in lithium ion batteries. To improve the poor electrical conductivity, many researches have been studied by carbon coating and composite method. In this study, cation substitution of beta LiVOPO4 by transition metal Zr was carried out via sol-gel method. Firstly, oxalic acid and V2O5 in stoichiometric ratio were dissolved in deionized water with magnetic stirring at 70˚C. After a clear blue solution formed, a mixture of stoichiometric NH4H2PO4 and LiNO3 was added to the solution while stirring for 4h and the green gel formed. Finally, the dried gel was decomposed at 300˚C for 4h and the obtained product was sintered at 500 ˚C for 4h in air. The structural properties of pristine and Zr-doped LiV1-XZrxOPO4 compounds were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Infra-red spectroscopy (IR) and electronic conductivity. And electrochemical performances were examined such as electrochemical impedance spectroscopy (EIS), and cyclic voltammetry (CV) and charge-discharge analysis (CD). Electrochemical results demonstrated that a proper amount of Zr-doping leads better discharge rate performance and cycle retention. To further understand the effects of Zr doping on the electronic structure of beta LiV1-XZrxPO4, First-principle calculations was performed. The results showed that Zr-doped does not changed beta LiVOPO4 crystal structure. And positively affects the electronic structure by lowering the band gap and increasing the DOS near the Fermi level.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-571**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Unzipped porous multi-walled carbon nanotubes by alkali activation for ultracapacitors with high energy density

한조아 권하나 노광철[1,*]

한국세라믹기술원 에너지소재센터 [1]한국세라믹기술원 에너지효율소재팀

Unzipped porous multi-walled carbon nanotubes (MWCNTs) with high specific surface area were prepared through alkali activation. Firstly, various pores were formed on the surface of MWCNTs after severe alkali activation. Subsequently, a longitudinally unzipped structure was obtained as the individual pores connected. In contrast with acid treatment to prepare unzipped CNTs, this akali activation is economical and scalable because it enables a one-step synthesis of unzipped and porous CNTs, simultaneously. As result of pore distribution by NL-DFT, the distribution of micro-meso pores showed evidence of unzipping because the peak for pore sizes

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-572**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of naphthoquinone derivatives and electrochemical performance for Li-organic flow batteries

신동선 홍성유[1,*]

UNIST 에너지 및 화학공학부 [1]UNIST 나노생명화학공학부

Redox flow batteries (RFBs) are highlighted for large energy storage system, because of increasing energy generation from intermittent renewable energy source, such as solar energy and wind power. Especially, nonaqueous redox flow batteries (NRFBs) are widely studied to overcome problem of low electrochimical window in traditional water based system. In organic electrolyte case, it has wide electrochemical window both low and high potential, so we may expect increase of energy and power density. Also, organic active materials; contrary to determinative kinds of inorganic metal ions, have diverse kinds of redox sites, furthermore each redox sites can be easily tuned and optimized by hundreds of functional groups for superior performance; such as higher voltage, stability, solubility, and etc. Herein we report novel 1,4-naphthoquinone derivatives, 2-phenyl-1,4-naphthoquinone (PNQ) and its methoxy group attached derivatives (mPNQ). The methoxy group can show electron-donating effect by the resonance stabilization also be electron withdrawing behavior because of inductive effect. Compounds can be synthesized with Suzuki-coupling reaction between 2-bromo-1,4-naphthoquinone and phenyl boronic acid series with high yield. And synthesized material's electrochemical characteristics are characterized by experimental and computational methods.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-573**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ionic Conduction and Solution Structure in Dimethyl Carbonate and Diethyl Carbonate Electrolytes

황순욱 김동휘 이호춘*

DGIST 에너지시스템공학

Further progress of the current lithium ion battery (LIB) can be achieved through fundamental understanding on the solvate structure and ion transport behavior which are closely related with ionics of the electrolytes. Our understanding on the ionics in the LIB electrolytes is far behind the current status of LIB technology. Specifically, it is still unclear why the ionic conductivities of dimethyl carbonate (DMC) -based electrolytes are much higher than diethyl carbonate (DEC) -based ones, although DMC and DEC are quite similar in their physicochemical properties. Here, the ion speciation in (1) single DMC and DEC solutions with various lithium salts and (2) ethylene carbonate (EC)-mixed solutions with changing EC mole fraction are investigated using Dielectric relaxation spectroscopy (DRS), Raman spectroscopy, and Pulsed field gradient-Nuclear Magnetic Resonance (pfg-NMR). Based on the complementary information of ionics provided by DRS and Raman, the compositional changes of ion species are examined as a function of salt concentration and the EC mole fraction. We found that both solvent-separated ion pair (SSIP) and contact ion pair (CIP) directly contribute to the increases of the dielectric constants and ionic conductivities of the solutions. In detail, the higher ionic conductivity of the DMC-based solution is ascribed to (1) higher portions of SSIP and CIP, and lower content of agglomerates in the case of single DMC and DEC solutions, and (2) higher dissociation and lower content of agglomerates in EC-mixed solutions. Furthermore, the diffusion coefficient of Li+, and PF6- measured by pfg-NMR shows higher values in the DMC-based solution than that of the DEC-based electrolyte.

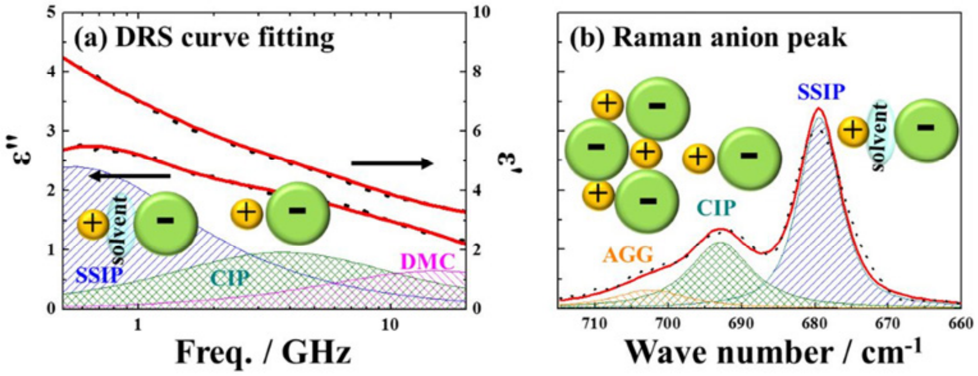


Figure 1 (a) Relative permittivity, ε'(ν), dielectric loss, ε''(ν), spectrum of 0.5M $LiAsF_6$ in DMC, showing the contributions from the various Debye process of ion pairs and solvent, (b) Raman spectra and anion peak separation of 0.5M $LiAsF_6$ in DMC.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-574**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of nitrogen doped graphene with $Co(OH)_2$ nanoflower for simultaneous detection of dopamine and uric acid

EJAZ AMMARA 전승원*

전남대학교 화학과

In current work, highly sensitive and stable electrochemical sensor for simultaneous detection of dopamine (DA) and uric acid (UA) have been constructed based on the nitrogen doped graphene (N-GO) decorated with $Co(OH)_2$ nanoflower. The N-GO-$Co(OH)_2$ is simply fabricated by chemical reduction method. Physicochemical analysis such as, scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS) have revealed successful doping of nitrogen on GO and fine dispersion of Co(OH)2 nanoflower on the surface of N-GO. The N-GO-$Co(OH)_2$ structure with the advantages of large surface area, excellent structure stability, and rich pore channels is used for facilitating the electron conductivity and their transfer. Combined with the dual effects of the N-doping and the excellent electrocatalytic activity of the $Co(OH)_2$ nanoflower, constructed sensor exhibits high electrochemical sensing activity with wide linear responses from 1μM to 1mM and 40 μM to 6mM for detection of DA, and UA respectively. In addition, N-Go-$Co(OH)_2$ composite also showed long-term sensing stability, reproducibility and excellent analytical response in urine for UA and DA detection. Furthermore, N-Go-$Co(OH)_2$ has shown a good anti-interfering behavior towards ascorbic acid (AA), serotonin (5-HT) and glucose (Glu). The N-GO-$Co(OH)_2$ composite manifests intriguing application potential as the candidate for the application of the electrochemical sensor for simultaneous detection of DA and UA.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-575**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile fabrication and characterization of Nb2O5 inverse opal nano architecture with significant beneficial photoelectrochemical properties

AR.Maheswari 강순형[1,*]

전남대학교 화학과 [1]전남대학교 화학교육과

Niobium oxide (Nb2O5) showing significant advancements in tailoring the promising n-type semiconductor photoelectrodes with relatively wide band gap (Eg = 3.4 eV) is of the much importance due to its wide range of catalytic activities including photodegradation of harmful organic contaminants and water photolysis, which is an advantage for environmental and energy issues. In particular, Nb2O5 has intensive interests in photoelectrochemical water splitting because of their unique optical properties and excellent qualification to be radiative centers and long term stability in aqueous medium which directly leads to the favourable results in photoelectrochemical water splitting. Herein, Nb2O5 inverse opal (IO) films were produced by the facile template assisted synthesis route on the opal template with diameter of 350 nm made through spin coating technique The photoelectrochemical behaviour of Nb2O5 IO films was surveyed by the linear sweep voltamograms in 0.1 M NaOH solution under solar illumination (AM 1.5 G), revealing that the photocurrent density of 2 mA/Cm2 vs RHE was obtained.The crystal structure, film morphology and photo physical behaviour of Nb2O5 IO photoelectrode were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), UV-Vis diffuse reflectance spectra (DRS) techniques. Furthermore, the morphological effect of Nb2O5 IO film as well as the effect of pore size of Nb2O5 inverse opals have been concisely investigated.Keywords: Nb2O5 inverse opal, Polystyrene opal template, Photoelectrochemical water splitting

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-576**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical microfluidic separation of circulating tumor cells in the blood samples

GurudattNanjanaguduGanesh 심윤보*

부산대학교 화학과

AC potential modulated microfluidic separation method coupled with an amperometric sensor was developed for the fast separation (

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-577**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A cathode material using radially aligned hierarchical columnar structure for high energy density as a sodium-ion batteries

유태연

한양대학교 에너지공학과

Lithium batteries currently dominate the secondary battery market because of their high energy and good power density. Recently, fossil fuel depletion and air pollution concerns have accelerated the development of mid- and largescale batteries for vehicles and energy storage devices. The recent launch of several types of electric vehicles powered by rechargeable lithium batteries has necessitated significant improvements in battery performance including higher capacity and power, longer life cycle and improved safety. Despite their feasibility, the mass production of such large-scale batteries would likely contribute to the future exhaustion of limitedlithium resources. This concern has led us to look for alternative systems to replace current lithium-related chemistries. Because of sodium's abundance in nature, sodium-based rechargeable batteries have recently received intensive attentions. Electrochemical insertion/extraction of sodium ion was introduced in the early 1980s but research has been directed towards lithium systems due to lithium's higher available energy. Provided that appropriate electrode materials can be discovered, substituting Na for Li should be accelerated due to the similar chemistries between Li and Na systems because Na is substantially less expensive than Li. Delivery of high capacity with good retention is a challenge in developing cathodes for rechargeable sodium-ion batteries. Here we present a radially aligned hierarchical columnar structure in spherical particles with varied chemical composition from the inner end (Na[Ni0.75Co0.02Mn0.23]O2) to the outer end (Na[Ni0.58Co0.06Mn0.36]O2) of the structure. With this cathode material, we show that an electrochemical reaction based on Ni2þ/3þ/4þ is readily available to deliver a discharge capacity of 157 mAh (g-oxide)1 (15mAg1), a capacity retention of 80% (125mAhg1) during 300 cycles in combination with a hard carbon anode, and a rate capability of 132.6 mAhg-1 (1,500mAg-1, 10 C-rate). The cathode also exhibits good temperature performance even at 20C. These results originate from rather unique

chemistry of the cathode material, which enables the Ni redox reaction and minimizes the surface area contacting corrosive electrolyte.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-578**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Advanced cathode Silver nanowire for Li-O_2 Batteries

강진혁

한양대학교 에너지공학과

In Li-O_2 batteries, precipitation of Li_2O_2 passivates the cathode's surface during charging, what terminates electrochemical reaction and limit the cell capacity. In the charging process, oxidation of the non-conductive Li peroxide precipitants requires high over-potentials, in which solution species may be readily oxidized. In order to address these shortcomings, many researchers tried to modify the morphology, size, and crystallinity of Li_2O_2 during its generation by electro-catalysis and the use of composite cathodes comprising nano-materials.Efforts have been made to decrease the overpotential at the formation and decomposition of Li_2O_2, by identifying catalysts that can control the morphology of Li_2O_2. Morphological control makes Li_2O_2 easier to decompose on oxygen evolution reaction (OER). Herein, we show that silver nanowires as cathode materials for Li–oxygen batteries. Silver nanowire (AgNW) greatly reduce the charging over-potential needed for OER at the solution/electrode interface and are more effective than silver nanoparticles (AgNP).AgNW deliver reversible Li_2O_2 formation/decomposition on discharge/charge with an average charging potential of ～3.4 V without electrolyte solution decomposition after 50 cycles. We confirmed that unique Li_2O_2 structure can promote the decomposition at low charge potential upon oxygen evolution reaction leading to high electrical efficiently of Li-air batteries up to 83.4%.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-579**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A simple fabrication of MWCNT interlayer for Lithium-Sulfur Batteries

김희민

한양대학교 에너지공학과

Rechargeable batteries are one of the prime approaches for electrical energy storage. The current lithium-ion battery technology based on transition-metal oxide cathodes and graphite anode have limited energy storage capacity, so there is immense interest to develop alternate high-capacity cathode and anode materials. Lithium-sulfur (Li-S) batteries are appealing in this regard as they offer a high energy density of 2500 Wh kg-1 when coupled with lithium-metal anode due to the large charge-storage capacity of sulfur. Moreover, sulfur is much more abundant, inexpensive, and non-toxic compared to the transition-metal oxide cathodes.There are several challenges with the Li-S batteries, such as low electrical conductivity of sulfur and the discharge product Li2S and the migration of dissolved polysulfides from the cathode to the anode, resulting in low efficiency and inadequate cycle life. Well-designed carbon-sulfur composites have been extensively explored to overcome these issues. In these strategies, sulfur was entrapped in carbon structures using porous carbon, carbon nanotubes (CNT), and hollow carbon spheres. Carbon backbone serves as the electron conducting path for sulfur and reduce polysulfide migration by trapping the polysulfides during cycling. However, polysulfide migration still occurs and cycle life is inadequate for practical applications. Manthiram group and other groups introduced the use of carbon-paper interlayers in between the sulfur cathode and the polymer separator or carbon-coated membrane and demonstrated high sulfur utilization with better cycle life due to the suppression of polysulfide diffusion to the anode and the serving of the carbon-paper interlayer as a pseudo-upper current collector.We present here the fabrication of an interlayer consisting of MWCNT and the electrolyte in a single fabrication process. Such MWCNT-electrolyte-paper interlayers are much more effective compared to the bare MWCNT-paper interlayer due to the fast ionic and electronic transport and a better interface between the sulfur cathode and the interlayer as well as between the separator and the interlayer.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-580**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mo2C nanoparticle on CNT composite for lithium-oxygen battery

곽원진

한양대학교 에너지공학과

Higher energy density of Li–O2 battery compared to conventional Li-ion battery and its environment friendly character make this system a promising energy storage system. In spite of great prospect, practical usage of Li–O2 battery system still has many challenges such as low energy efficiency, poor rate capability and a poor cycle life. These problems are mainly attributable to excessive accumulation of discharge products (Li2O2), which induce poor reversibility and high polarization when they decompose during charging. Consequently, the number of operating cycles for Li–O2 batteries cannot yet match those of Li-ion batteries. Moreover, the energy efficiency (< 80%) of the present Li–O2 battery system is also too low. To improve the performance of Li–O2 battery systems, a key factor is finding ways to enhance the catalytic activity of the cathode for formation and decomposition of Li2O2, which is critical to decrease the polarization and increase the reversibility. Herein, we introduce well dispersed molybdenum carbide nanoparticles onto carbon nanotubes (Mo2C/CNT) as a cathode material for Li–O2 batteries. Mo2C could be a good catalyst for the oxygen evolution reaction (OER) in Li–O2 batteries and the carbon nanotubes could help the Mo2C nanoparticles be an ORR catalyst due to its electrical conductivity. In this report, a Mo2C/carbon nanotube composite as a cathode is demonstrated to reduce high over potentials during charge and improve the cycling performance of Li–O2 batteries.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-581**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Problems of lithiated anode in Li-air batteries

이선화

한양대학교 에너지공학과

Lithium oxygen battery is attractive battery system which can make high energy density for next generation. However, even if the many researches have been progressed for years,1-4 the works about substitution of Li metal which has inherent limitation of stability and long term cycling property was terribly deficient. Here in, our group clearly demonstrate the ambiguously unsolved problem of lithium oxygen full cell system using alternative anode (lithiated Si-CNT composite) for lithium metal by XRD and SEM analysis. The amount of lithium source in alternative anode is limited compared to quasi infinite amount of Li source in Li metal. The returning lithium ion at the charge forms the lithium hydroxide which passivates the anode by side reaction with moisture in electrolyte and from outside. Side reactions, leading to the formation of LIOH at the anode site caused loss of the Li source, resulting in decreased potential and poor cycle of the Li-O2 full-cell system. Although the Li-O2 full-cell without lithium metal could be a good area for practical Li-O2 battery work in terms of safety, it is not viable without solving the Li loss problem. Our results could be helpful for further research into Li-O2 full-cell systems, and this issue could constitute a fundamental theme for future practical Li-O2 battery systemsReferences(1)M. M. O. Thotiyl, S. A. Freunberger, Z. Peng, P. G. Bruce, J. Am. Chem. Soc., 2013, 135, 494-500.(2)B. M. Gallant, R. R. Mitchell, D. G. Kwabi, J. Zhou, L. Zuin, C. V. Thompson, Y. S. Horn, J. Phys. Chem. C, 2012, 116, 20800-20805.(3)V. S. Bryantsev, V. Giordani, W. Walker, M. Blanco, S. Zecevic, K. Sasaki, J. Uddin, D. Addison, G. V. Chase, J. Phys. Chem. A, 2011, 115, 12399-12409.(4)D. Sharon, V. Etacheri, A. Garsuch, M. Afri, A. A. Frimer, D. Aurbach, J. Phys. Chem. Lett., 2013, 4, 127-131.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-582**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Potentiostatic activation of as-made graphene electrodes for high-rate performance in supercapacitors

<u>KRISHNAN SENTHILKUMAR</u> 표명호*

순천대학교 인쇄전자공학과

Supercapacitors are electrochemical charge-storage devices, the electrochemical performance of which fills the gap between traditional electrolytic capacitors and state-of-the-art secondary batteries. The conventional method used to accomplish this in a supercapacitor is to implement an electrode material with a high specific surface area, in which the charge-storage occurs via electric-double layer (EDL) formation at the electrolyte/electrode interface. Graphene (one-atom-thick sp^2 carbon sheets) with an incomparably high theoretical surface area (~2600 $m^2 \cdot g^{-1}$) is a fascinating candidate for high-performance EDL capacitors. The high electrical conductivity and excellent electrochemical stability of graphene also makes this notion plausible. Despite the theoretical prediction of high capacitance (ca. 550 $F \cdot g^{-1}$), however, the experimentally obtained capacitance in graphene-based EDL capacitors has been limited, which is due mainly to face-to-face restacking between the graphene layers in the electrode. In order to overcome this hurdle, we presented a strategy based on electrochemical water oxidation. A thermally expanded graphene oxide (EGO) electrode is electrochemically activated to simultaneously introduce electrolyte-accessible mesopores and oxygen functional groups. The former is produced via O_2 evolution and the latter is incorporated by the intermediate hydroxyl radicals generated during the potentiostatic oxidation of H_2O in 1 M H_2SO_4 at 1.2 V (vs. Ag/AgCl). When applied as a supercapacitor, the potentiostatically treated EGO (EGO-PS) shows significant enhancement in an electric-double layer (EDL) process with a noticeable Faradaic reaction and delivers high capacitance at fast charge/discharge (C/D) rates (334 $F \cdot g^{-1}$ at 0.1 $A \cdot g^{-1}$ and 230 $F \cdot g^{-1}$ at 50 $A \cdot g^{-1}$). EGO that is oxidized potentiodynamically (EGO-PD) or that is subjected to successive potential pulses shows negligible enhancement in EDL currents, which indicates the importance of hydroxyl radical concentration for simultaneous functionalization and microstructure control of graphenes. The potentiostatic post-treatment presented here is a convenient post-treatment strategy that could be used to readily increase capacitance and simultaneously improve the high-rate performance of carbon-based electrodes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-583**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparison of the Catalytic oxidation reaction of Dopamine on Environmentally Friendly Reduced Graphene oxides by Chemical and Electrochemical Method

유준희 심수진 김태현*

순천향대학교 화학과

Graphene oxide (GO) has been widely used in a variety of applications, particularly as a sensing material due to its high carrier mobility, large surface area and catalytic properties. However, preparation of reduced GOs often, require toxic and/or explosive reducing agents, such as commonly-used hydrazine hydrate and sodium borohydride. Consequently, various efforts have been made for green preparation of GOs. Here, we have prepared environmentally friendly reduced GOs by chemical reduction via ascorbic acid and electrochemical reduction. The chemically and electrochemically reduced GOs have been modified onto glassy carbon electrode to investigate the feasibility of electrochemical sensor for dopamine and compare the catalytic oxidation reaction of dopamine. The modified electrodes were characterized using Raman spectroscopy, contact angle measurements, and electrochemical methods.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-584**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Simple preparation and electrochemical performance of graphene oxide/carbon nanotubes composite electrode

손영래 박수진*

인하대학교 화학과

Graphene oxide/carbon nanotube (GO/CNT) composite electrode was prepared by a simple drop casting and evaporation of solvent. CNT can be dispersed in water using GO because GO plays a role in dispersing CNT in aqueous solution as a dispersing agent. Thus, GO/CNT composite electrode can be simply and environmentally friendly fabricated from stable dispersion of GO/CNT in water. X-ray diffraction (XRD) and scanning electron microscope (SEM) were used to investigate the structural properties and morphologies, respectively. The electrochemical measurements of GO/CNT composite electrode were conducted by cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD). Compared with GO, It was found that the specific capacitance of GO/CNT composite electrode was enhanced by CNT.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-585**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of the structure stability according to Ti substitution at V sites in α-LiVOPO4

이성훈 류광선*

울산대학교 화학과

LiVOPO4 has high potential of 4.0 V and it has a theoretical capacity of 166 mAh g-1. In addition to this, it appears the high theoretical energy density (664 Wh/kg) as against the 578 Wh/kg for LiFePO4. Based on the spatial arrangement of VO6 octahedral and PO4 tetrahedral units, LiVOPO4 exists different crystallographic phases such as α-, β-. γ-. δ-. ε-, ω- LiVOPO4. Triclinic α-LiVOPO4 among them has magnificent electrochemical performance. This material has poor intrinsic electronic conductivity and ionic conductivity. Various effective approaches have been introduced to improve the both conductivity, including coating, particle size reduction, doping with alien cations. Among the above approach, alien cations doping have effects of crystal stability, the transportation of electron and Li ion.In this study, we had substituted Ti at V sites in α-LiVOPO4 to show the above effects. This material was synthesized by the sol-gel method. The starting materials used ammonium vanadate, lithium hydroxide, ammonium dihydrogen phosphate, and titanium oxide. The structure analysis of synthesized LiVOPO4 and impurities formation were confirmed through the XRD and FT-IR measurement. Also, SEM (Scanning Electron Microscopy) and EDS (Energy dispersive X-ray spectroscopy) measured to confirm the particle size of synthesized LiVOPO4 and distribution of atoms. And local structure such as bond length, oxidation state, and parameter of unit cell was confirmed by rietveld refinement and XAFS (X-ray Absorption Fine Structure). The Electrochemical Li ion intercalation performances such as EIS (Electrochemical Impedance spectroscopy), CV (Cyclic Voltammetry), CD (charge-discharge), rate capability also evaluated as the cathodes.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-586**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anatase TiO2 nanoparticles embedded on carbon nanotubes for sodium battery

<u>최민재</u>

한양대학교 에너지공학과

The main disadvantage of using transition metal oxides for Na+-ion batteries is the sluggish kinetics of insertion of Na+ ions into the structure. Here, we introduce nanosized anatase TiO2 that is partially doped with fluorine (TiO2F) to form electro-conducting trivalent Ti3+ as an ultrafast Na+ insertion material for use as an anode for sodium-ion batteries. In addition, the F-doped TiO2F is modified by electro-conducting carbon nanotubes (CNTs) to further enhance the electric conductivity. The composite F-doped TiO2 embedded in CNTs is produced in a one-pot hydrothermal reaction. This yields a high electric conductivity of approximately 5.8 S cm-1 . The first discharge capacity of the F-doped TiO2 embedded in CNTs is approximately 250 mA h (g-oxide)-1, and is retained at 97% after 100 cycles. As expected, a high-rate performance was achieved even at the 100 C discharging rate (25 A g-1).

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-587**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An amperometric nanobiosensor using a biocompatible conjugate for the in vitro detection of nicotine induced cellular release of BDNF

AKHTARMAHMOODHASSAN 심윤보*

부산대학교 화학과

A nonenzymatic amperometric immunosensor was developed to detect brain-derived neurotrophic factor (BDNF) in cancerous cells. The sensor was constructed by covalently immobilizing the antibody Ab1 onto functionalized surface of 4-[2,2':5',2''-terthiophen]-3'-yl) benzoic acid (pTTBA) and gold nanoparticles. Ab2 and toluene blue O were attached on self-assembled gold nanoparticles and polymer 4-([2,2':5',2''-terthiophen]-3'-yl) benzoic acid (pTTBPA) to prepare the bioconjugate nanocomposite. Morphology and performance of sensor probe were examined by field emission scanning electron microscopy (FE-SEM), X-ray photoelectron spectroscopy (XPS), quartz crystal microbalance (QCM), electrochemical impedance spectroscopy (EIS), and electrochemical techniques. Reliability of the proposed system was evaluated by detecting the extracellular escalated BDNF level in cancerous cell line in vitro with the induced effects of anti-apoptotic agent, nicotine.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-588**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Graphite Oxide as nano-template for the Synthesis of Cobalt Oxide Hybrid Electrodes for Supercapacitor Applications

ANTHONISAMY NIRMALESH NAVEEN 표명호*

순천대학교 인쇄전자공학과

In this work, we have used two different carbon-based graphene oxide (GO) and graphite oxide (GTO) which have typically planar arrangement of sp^2-bonded carbon atoms, as nano-template for the synthesis of cobalt oxide hybrid composites for supercapacitors. Hybrid electrodes prepared by decoration of metal oxides within GTO are expected to show superior charge transfer rate and high cycling stability, owing to their high electrical conductivity and mechanical strength. We used GTO to avoid random restacking of graphene sheets and particle aggregation occurring during synthesis that severely hinders the electrode performance. In this regard, GTO with pre-aligned nature can be an effective nano-template for metal oxide encapsulation. Spinel formation of cobalt oxide in synthesized Co_3O_4/rGTO and Co_3O_4/rGO composite (r-stands for reduced) were determined from XRD and XPS measurements. Imaging techniques reveal the well dispersion of nano-sized cobalt oxide particles within the graphitic layers of Co_3O_4/rGTO composite in contrast to the particle aggregation found on top of the randomly stacked graphene sheets in Co_3O_4/rGO. Cyclic voltammetry study unraveled the typical faradaic redox mechanism of the composite material in 3 M KOH electrolyte. Highly reversible twin redox peaks typical of Co_3O_4 structure appeared in the CV curve of 20 mM Co_3O_4/ rGTO which depicts the excellent charge transfer rate and superior accessibility of the electro-active species. Co_3O_4/rGTO hybrid electrode exhibited a high specific capacitance of 606 $F.g^{-1}$ at 5 $mV.s^{-1}$ as compared to 340 $F.g^{-1}$ by Co_3O_3/rGO. Remarkable cycling retention of 84% was observed for Co_3O_4/rGTO at the end of 10000 cycles is far superior to Co_3O_4/rGO composite that displayed only 26% retention. High rate performance and cycling stability of Co_3O_4/rGTO composite can be understood from the negligible charge transfer resistance and buffering effect of well aligned graphite layer architecture, as can be inferred from the EIS and morphology study respectively.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-589**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Change of the polarization resistance during an electrochemical-chemical reaction

장병용* 정휘석 이설혁

부경대학교 화학과

Here we present an electrochemical simulation results comparing voltammetric current and resistance of a coupled reaction of electrochemical and chemical processes over a potential scan. For this work, the finite element method is used that are frequently used for voltammetry but rarely for impedance spectroscopy. Here, this method is used for simulation of a complex reaction where a heterogeneous faradaic reaction is followed by a homogeneous chemical reaction. By tracing the current and its polarization resistance, I studied their relationships to be explained in terms of rate constants of charge transfer and chemical change. An unexpected observation was made that even though the resistance is increased by the rate of the following chemical reaction, the current can be increased due to the potential shift of the resistance made by the proceeding faradaic reaction. This result telles that FEM-based resistance simulation can be applied to understand a complex electrochemical reaction. Until now, resistance simulations are mostly based on equivalent circuits or complete mathematical equations and have limitations to find proper models. However, this method is based on the first-principles, and is expected to be complementary to the other simulation methods.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-590**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synaptic Cell Adhesion Molecules for Synapse-Electrochemistry

전주희 오민아 정택동*

서울대학교 화학부

Neuronal cells have cellular gap junctions called ‘synapses’ between two adjacent neurons where the transmission of electrochemical information takes place. Research on various events occurring at the synaptic cleft, however, has been limited owing to the poor spatial accessibility to extremely narrow gap, ~20 nm wide. To approach the electrochemical events at the synapse in another direction, we made attempts to induce synapses directly on the artificial surface including electrodes instead of conventional neuroelectrochemical system, e.g. inserting a sharp nano-electrode into a synaptic cleft. To that end, we engineered neuroligin 1 (NL1), a synaptic cell adhesion molecule (CAM), which is known to drive the formation of presynapses. NL1 was biotinylated following an in vivo process to be immobilized on streptavidin-coated surface. Such engineered proteins on microbead substrates brought about the glutamatergic (excitatory) pre-synaptic differentiations when co-cultured with primary hippocampal neurons. In addition to excitatory synaptic CAM, we were able to prepare inhibitory one, Slitrk3, on the same kind of microbeads. Microfluidic chip allows us to make synaptic CAM modified beads exposed to pure axons from the embryonic hippocampus neurons seeded on PDK coated glass surface. We confirmed the engineered post-synaptic CAMs are capable of inducing artificial synapse through which persistent and durable information transmission takes place between live neurons and electronic devices. With this new system, we would be able to do real electrochemistry at artificial synapse and see what happens inside the synapse-electrode interface, suggesting an innovative breakthrough in neuroelectrochemistry.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-591**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ultrasensitive Nanoimmunosensor Based on Non-Covalent Functionalized Graphene Oxide Platform and Carbon Nanotubes Bounded Ferritin Labels

Akter Rashida 정봉진 **Md. Aminur Rahman**[*]

충남대학교 분석과학기술대학원

An ultrasensitive electrochemical nanoimmunosensor for a breast cancer biomarker carbohydrate antigen 15-3 (CA 15-3) was fabricated using non-covalent functionalized graphene oxides (GO/Py-COOH) as sensor platform and multiwalled carbon nanotube (MWCNTs)-bonded numerous ferritin as labels. The immunosensor was constructed by immobilizing a monoclonal anti-CA 15-3 antibody on the GO modified cysteamine (Cys) self-assembled monolyer (SAM) on an Au electrode (Au/Cys) through the amide bond formation between the carboxylic acid groups of GO/Py-COOH and amine groups of anti-CA 15-3. Secondary antibody and ferritin conjugated MWCNT bioconjugates (Ab2-MWCNT-Ferritin) were prepared through the amide bond formation between amine groups of Ab2 and ferritin and carboxylic acid groups of MWCNTs. The detection of CA 15-3 was achieved through monitoring the ferritin catalyzed hydrogen peroxide reduction at the GO/Py-COOH-based sensor probe. The GO/Py-COOH-based sensor probe and Ab2-MWCNT-Ferritin bioconjugates were characterized using various techniques. Using differential pulse voltammetry (DPV), CA 15-3 can be selectively detected as low as 0.01 ± 0.07 U/mL in human serum samples with excellent stability, which demonstrated that the proposed nanoimmunosensor has potentials in proteomic researches and diagnostics.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-592**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Novel Electrochemical Biosensor Based on Quantum Dot Dissolution for a PMI Marker Detection

정봉진 **Akter Rashida Md. Aminur Rahman***

충남대학교 분석과학기술대학원

GAPDH (GD) is a protein which can be found frequently at the human body such as saliva and kidney and it can be utilized in forensic science such as postmortem interval (PMI) detection. GD is very important as its concentration decreases with time after death. This characteristic of GD protein can be utilized as a biomarker for developing a PMI biosensor system in saliva. The PMI biosensor was fabricated by immobilizing a monoclonal anti-GAPDH antibody on the functionalized cadmium selenide (CdSe) quantum dots (QD), which were attached on the self-assembled monolayer (SAM) of cysteamine containing graphene oxide (GO). The GAPDH detection was made through the dissolution of the surface attached CdSe QD by hydrogen peroxide, which was generated through the glucose oxidase (GOx) catalyzed β-glucose oxidation. GOx was used as an enzymatic label that was conjugated to GD protein through glutaraldehyde cross-linking. For enhancing the sensitivity by reducing the sensing layer, we performed the competitive assay in which GD-GOx conjugates and free-GD competed for binding to the active sites of antibody. The current response resulted from the CdSe dissolution was found to be decreased with increasing concentration of free GD and was proportional to the free-GD concentration. Thus, it was possible to quantify the free GD with this strategy and differential pulse voltammetry (DPV) technique was used to determine the analytical characteristics such as detection limit (DL) and linear dynamic range of GD detection, selectivity, stability, and the real sample analysis for the GD detection.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-593**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Water oxidation activity improvement of $Ni(OH)_2$/NiOOH electrocatalyst on Carbon based supports

이광익 황윤정*

한국과학기술연구원(KIST) 청정에너지 연구센터

물 전기분해는 친환경 연료인 수소 생산에 중요한 방법이나 이 과정의 산소발생반응은 큰 과전압이 필요하다. 그래서 이 느린 반응속도를 극복하기 위해 물산화 전기화학 촉매는 신재생에너지 분야에서 중요한 연구분야이다. 최근의 물산화 촉매는 산화코발트 또는 니켈-철 합금 촉매와 같은 낮은 가격과 주변에 풍부한 원소들을 이용한 연구가 이루어지고 있다. 많은 연구자들이 촉매재료의 낮은 가격에 관심을 가짐에도, 촉매의 성능을 향상 연구에 있어서는 비싼 Au 이 널리 이용되고 있다. 이 연구에서는 $Ni(OH)_2$/NiOOH 촉매는 Au 기판을 대신하여 저가의 탄소 소재 기판을 사용하였으며, 질소로 도핑된 탄소 지지체를 사용할 경우, Ni 촉매 활성에 끼치는 영향에 대해서 연구하였다. 특히, Fe-N-C 기판에서 과전압이 감소하는 등 성능이 향상됨이 관찰되었다. 일반적으로 1M KOH 전해질에서 Au 기판 위의 $Ni(OH)_2$/NiOOH 촉매의 과전압은 10 mA/cm^2 에서 360mV 이나 Fe-N-C 기판 에서는 310mV 이 달성되었다. XPS 및 전기화학적 측정 결과는 Ni-Fe 의 합금 효과가 아니라 지지체와 촉매 사이의 상호 작용에 의해 Ni (oxy)hydroxide/Fe-N-C 의 촉매 활성이 향상되었음을 제시한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-594**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gold Nanostructures co-deposited from M13 Virus Mixed Electrolyte as a Biosensor

서예지 Shanmugam Manivannan 김규원*

인천대학교 화학과

We developed a novel biosensor electrode for nitrite ions. Gold dendritic nanostructures (Au-DNs) are directly electrochemically co-deposited from 4E peptides engineered M13 virus (M134E) mixed electrolyte on to the ITO electrode. The M134E could specifically nucleate Au precursor, which enable the efficient growth of dendritic nanostructures, whereas such structures were not obtained in the presence of wild-type M13 virus. The structural features of the Au-DNs and their interfacing mechanism with ITO electrode are characterized by SEM, EDX and XRD analysis. The growth mechanism of Au-DNs at ITO electrode has been elucidated by SEM measurements. The M134E induces the formation and plays a crucial role in shaping the dendrite morphology of Au nanostructures. Biosensor electrode constructed using Au-DNs modified electrode for nitrite ions and found improved sensitivity relative to the sensor electrode prepared from wild-type M13, Y3E peptides engineered M13 and without M13. Our novel biosensor fabrication can be extended to other metal and metal oxides and its application might be useful to develop novel biosensor for variety of biomolecules.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-595**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrodeposition of Virus–Platinum Nanohybrids for Methanol Oxidation Reaction

Shanmugam Manivannan 윤진아 서예지 김규원*

인천대학교 화학과

M13 virus (M13) as scaffolds has a major appeal, owing to their mono-dispersed, fibrillar morphology and engineerable surface reactive sites. We developed a facile for energy application. Platinum nanostructures are directly co-deposited from a wild-type M13 and two different engineered M13 mixed electrolytes onto ITO electrodes. The engineered M13 with 4E peptides could specifically nucleate Pt precursor, which enable the efficient growth of teeth-like structures at the ITO electrode. The electrocatalytic activity of the resulting biocatalyst toward methanol oxidation in alkaline medium was investigated and found enhanced mass activity relative to the catalyst prepared from wild-type M13, Y3E peptides engineered M13 and without M13. Our novel biocatalyst fabrication can be extended to other metal and metal oxides and its application might be useful to develop novel clean and green energy generating and storage materials.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-596**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Ultrasonic-assisted Preparation of BiVO4 Nanocrystals for Photoelectrochemical Water Oxidation

박기상 김지현 남기민*

목포대학교 화학과

Photocatalysis is a light-driven chemical process over the surface of a semiconductor that can produce hydrogen from water. Among semiconductors, BiVO4 as an n-type semiconductor is one of the most well-known photocatalysts under visible light irradiation due to its comparatively small band gap (Eg = 2.4 eV). Despite the considerable attention in the photoactive BiVO4, it is known to be inactive kinetics of holes, retard charge transfer at the interface of semiconductor and electrolyte, and rapid electron-hole recombination. Here, the BiVO4 thin film was successfully fabricated on fluorine-doped tin oxide (FTO) substrates by ultrasonic-assisted chemical method. A high photocurrent density of 1.5 mA/cm2 under UV-vis light illumination and 0.6 mA/cm2 under visible light illumination ($\lambda \geq 425$ nm) was obtained at 0.6 V vs Ag/AgCl, which is significantly higher than those from various other BiVO4 thin films.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ELEC.P-597**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Sonochemical Synthesis of ZnO/ZnS Core/shell Nanorods for Photoelectrochemical Water Oxidation

오경희 임태완 남기민*

목포대학교 화학과

Artificial photosynthetic systems are promising approaches to convert sunlight into chemical fuels. The most popular strategy is photoelectrochemical (PEC) water splitting to produce hydrogen sustainably. Metal oxide composites, typically comprising a primary photon absorbing semiconductor with a secondary semiconductor that may play a number of assisting roles, are constructed using various materials to elucidate the processes of electron-hole separation and charge transport through the composite. Here, the ZnO/ZnS Core/shell Nanorods was successfully fabricated on fluorine-doped tin oxide (FTO) substrates by ultrasonic-assisted chemical method. A high photocurrent density of 0.6 mA/cm2 under UV-vis light illumination was obtained at 0.6 V vs Ag/AgCl, which is significantly higher than the ZnO nanorods.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-598**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

자유학기제 주제선택 활동기반 화학 프로그램 개발

최희 백성혜[1,*]

충청북도교육청 율량중학교 [1]한국교원대학교 화학교육과

본 연구는 2016 년 전국의 중학교에서 전면시행 중인 자유학기제 주제선택 활동에 활용할 수 있도록 개발하였으며 학업의 부담 때문에 학문의 본질에 대하여 깊게 생각할 기회가 없었던 학생들에게 다양한 사고를 펼칠 기회를 제공하고 생각과 소통하는 힘을 기르는 것을 목적으로 한다. 본 프로그램은 '물질의 상태', '용해', '산·염기', '산화·환원' 등을 소재로 선정하여 총 16 차시(8 개 블록, 1 블록당 2 차시)로 개발하였다. 각 소재의 지식을 학습하기보다는 NOS 를 학습하는데 초점을 두었으며, 학습 과정은 논의 활동이 중심이 된다. 평가는 학생들이 소통의 자세를 익히고 논의활동의 문화가 자리 잡을 수 있도록 대인관계 차원의 평가항목을 넣었으며, 이러한 논의 활동 속에서 자신의 사고를 성찰하도록 개인적 차원의 평가항목을 구성하였다. 또한 수업 속 활동이 지식에만 그치지 않고 학생들에게 사회적인 의미까지 확장될 수 있도록 사회, 국가, 공동체와의 관계 차원을 구성하였다. 이를 통해 자유학기제가 지난 후 다시 정규 교육과정으로 복귀되었을 때, 학력의 단절이나 저하의 우려를 극복하고, 오히려 그 학문의 근본에 대한 이해를 높이고 학문을 바라보는 시각을 새롭게 바꾸어 줄 것이다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-599**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

학습발달과정(Learning Progression) 기반의 자유학기제 주제선택 활동 부력 교육프로그램 개발

김성기 백성혜[1,*]

전남과학고등학교 [1]한국교원대학교 화학교육과

중학교 과정 중 한 학기 동안 학생들이 시험 부담에서 벗어나 꿈과 끼를 찾을 수 있도록 교육과정을 유연하게 운영하는 자유학기제는 2013 년 2 학기부터 시범적으로 적용되었으며, 2016 년 전국의 중학교에 전면시행되었다. 본 연구는 자유학기제 주제선택 활동에 활용될 수 있는 물리교과 기반의 프로그램을 개발하였다. 본 프로그램은 NGSS 를 기반으로 하여 관통개념을 경험할 수 있는 '부력'을 소재로 선정하였으며 총 16 차시(8 개 블록, 1 블록당 2 차시)를 개발하였다. 각 블록마다 자연 현상을 과학적으로 바라보는 눈을 가질 수 있는 활동과 이와 관련된 진로활동 및 이를 통한 과학 학문 그 자체의 아름다움을 경험하도록 구성하였다. 이를 통해 자유학기제가 지난 후 다시 정규 교육과정으로 복귀되었을 때, 학력의 단절 이나 저하와 같은 우려를 극복하고 오히려 그 학문을 단순히 암기하기 보다는 근본을 이해하도록 탐구하는 기폭제가 될 것이다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-600**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

산-염기 이론들의 관계에 대한 교사들의 인식 유형화 및 요인 분석

박철용 최희[1] 김성기[2] 백성혜[3,*]

천안중학교 [1]충청북도교육청 율량중학교 [2]전남과학고등학교 [3]한국교원대학교 화학교육과

학생들이 가지는 대안 개념의 근원 중 하나가 교사의 대안개념이라는 점에서 교사의 올바른 과학적 개념과 이해는 학생들을 지도하는데 필수적인 요소이므로 교사의 개념에 대한 인식을 알아보는 것은 의미가 있다. 그래서 본 연구에서는 Arrhenius, Brønsted-Lowry, Lewis 산 염기 이론의 관계에 대한 인식을 알아보고 이러한 인식의 요인을 밝히는 연구를 하였다. 이를 위해 K 대학교 대학원 과정에 있는 24 명의 교사를 대상으로 3 가지 산-염기 이론에 대한 교사인식 및 요인을 분석하였다. 연구 결과 산-염기 이론에 대한 교사들의 인식은 3 가지 유형으로 분류되었다. 이 3 가지 유형의 요인을 분석한 결과 2 가지 요인을 발견할 수 있었다. 첫 번째 요인은 초점을 물질 자체로 보는지 과정으로 보는지로써, 이에 따라 산-염기에 대한 분류가 달랐다. 두 번째 요인은 정의에 대한 개인적인 언어적 해석의 차이였다. 교사들은 이론의 설명 내용 중 일부분에 초점을 맞추어 다양하게 서로 다른 해석을 함을 확인할 수 있었다. 이 연구의 결과는 앞으로 교과서를 개발하거나 예비교사 교육을 수행할 때 혹은 교사가 학생들을 지도할 때 고려하여야 할 요인으로 중요한 의미를 갖는다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-601**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

고등학교 화학과 대학교 일반화학 교육과정의 연계성 분석

백은숙 홍훈기*

서울대학교 화학교육과

과학교육의 국제 비교 평가의 결과를 보면, 학생들의 과학성취도가 초등학교에서 중학교, 고등학교로 갈수록 낮아지고 과학적 태도가 긍정보다는 부정적인 부분이 더 많아지는 것으로 나타난다. 과학 교육 내용을 선정하고 조직할 때, 초·중·고등학교까지 학습자의 인지적 발달 수준에 따라 일관성 있게 교육하며 대학교육까지 연관성을 가지도록 계획하는 것이 필요하다. 연계성 분석은 수업 활동과 과학 교육에 대한 방향과 방법을 제시하기 위한 것이다. 본 연구의 목적은 현행 교육과정의 고등학교 화학과 대학교 일반화학의 교육과정 내용 사이의 연계성을 분석하는 것이다. 한국과학창의재단에서 개발한 「과학교육 내용표준」의 핵심내용지식을 기준으로 내용 분포를 분석한다. 핵심내용지식은 물질의 구조, 물질의 성질, 물질의 변화로 구성된다. 이를 기준으로 고등학교 화학 교과서와 대학교 일반화학 교재의 연계성을 분석한다. 이 결과를 바탕으로 2015 개정 교육과정이 교육현장에 성공적으로 적용되기 위한 발전 방안과 시사점을 제시한다.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-602**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

STEAM 연구학교 프로그램에 제시된 핵심역량 분석

최재민 백성혜*

한국교원대학교 화학교육과

창의적 인재를 양성을 위하여 STEAM 교육의 필요성이 제시되고 OECD 에서 핵심역량을 강조하면서 교육과학기술부에서는 STEAM 교육을 핵심역량 위주로 재구조화하는 교육정책을 제안하고 있다. 본 연구는 STEAM 연구학교에서 실시한 STEAM 프로그램에 제시된 핵심역량을 분석하였다. 또한 STEAM 프로그램 제작에 있어 기본 틀이 되고 있는 STEAM 학습 준거틀에 따라 각 단계에서 중요시 되는 핵심역량이 무엇인지 파악하고, 교사들이 직접 제작한 STEAM 프로그램이 STEAM 학습 준거틀에 따라 적절한 핵심역량을 반영하고 있는지에 대하여 분석하였다. 이를 통해 교사들의 핵심역량 중심의 STEAM 프로그램 개발 역량 강화를 위한 방향성 제시하고 STEAM 학습 준거틀에 따라 강조되어야 하는 핵심역량이 무엇인지 밝혀 보다 구체적인 STEAM 교육 프로그램 개발을 위한 가이드라인 제공할 수 있을 것이다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-603**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

융합교육프로그램이 공기 조성에 대한 교사들의 인식 및 PCK에 미치는 영향

송민규 백성혜[1,*]

계룡고등학교 화학 [1]한국교원대학교 화학교육과

지식 정보화 시대에 맞추어 새로운 기술을 창출할 수 있도록 문제 중심의 학습 형태 적용으로 창의적 융합 인재양성 필요(노상우, 2012)하며 앞으로의 교육은 실제 문제를 해결하는 새로운 지식의 생성으로 확장되어야 하므로 통합교육과정, 융합 학문적 교육과정이 요구된다(이승우 외, 2011). 이를 위한 융합교육은 통합적 관점을 통해 사물과 세계를 총체적으로 이해 할 수 있게 함으로써 창의적 문제해결능력을 갖춘 인재 양성에 적합(홍병선, 2009)하며, 다양한 경험 습득으로 문제 속 여러 이질적인 요소들을 하나로 융합해 내는 능력과 태도를 키울 수 있다(홍성욱, 2012). 이 같은 교육적 요구 속에서 교사는 앞으로 전통적 수업에서 지식 전달 역할이 아닌 새로운 교육적 패러다임을 제시해야하고(T. Wang, 2009) 교과내용을 재구성하여 지도하는 능력이 요구된다(백성혜, 2013). 특히, 현재 과학 교과서 제시된 대기 조성과 관련된 과학 개념이 단절적으로 제시되어있고 융합적으로 사고하기에 어려움이 있으므로(강원미, 2016; 윤소희, 2016), 이를 개선하기 위해 과학 교사들에게 융합교육프로그램 제공하고 그들에게 유의미한 인식변화와 대기 조성 과학 개념 영역과 관련된 PCK 신장을 이끌어낼 수 있다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-604**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

10년의 약속: 한국 과학교사들의 동티모르 봉사활동

한재영* 임성민[1]

충북대학교 사범대학 화학교육과 [1]대구대학교 과학교육학부

‘동티모르에 또 올 건가요?’, ‘그걸 왜 묻나요?’, ‘아무도 동티모르에 다시 오지 않아요.’ 한국 과학교사들은 동티모르에 10 년간 가서 봉사활동을 하기로 약속하였고, 2016 년까지 결국 그 약속을 지켰다. 이 연구는 ‘문화역사활동이론과 자기 연구를 통한 과학교사의 해외 봉사활동 질적 연구’의 일부로 동티모르 봉사활동의 변화 과정을 분석하였다. 문화역사활동이론에서는 하나의 활동체계를 주체, 객체(결과물), 도구, 커뮤니티, 규칙, 노동 분업으로 구분하여 분석한다. 10 여년간 동티모르 교사교육 봉사활동에 참여한 과학교사에 대한 면담, 활동 자료집, 연구자의 봉사활동 참여 일지, 과학교사가 쓴 글 등을 분석의 기초 자료로 삼았다. 봉사활동의 주체는 2004 년 과학교사 1 인에서 2016 년 과학교사 15 명, 대학교수 2 명, 대학생 1 명, 치과의사 1 명, 간호사 2 명 등으로 확장되었다. 객체(결과물)도 2004 년 동티모르 학생을 대상으로 한 시범이나 과학 수업에서 2016 년 과학 교사를 대상으로 한 실험 교육, 과학쇼, 소규모 과학축전, 치과 치료 등으로 확장되었다. 도구는 초기에 한국에서 가지고 가는 실험 재료와 기자재를 위주로 하였지만, 이후 동티모르에서 구할 수 있는 재료를 최우선하는 방향으로 변하였고, 언어 문제를 해결하기 위하여 자료집을 한글과 영어에서 현지어인 떼뚬어로까지 번역하여 제작하였으며 실험 과정을 보여주는 사진이나 그림 중심의 포스터를 만들기도 하였다. 커뮤니티에는 동티모르의 팔로모 신부, 동티모르 한국 대사, 동티모르 교사, 학생, 교육청 인사, 공항 직원 등이 포함되는데, 이들 구성원은 봉사활동을 지원하기도 하며 방해하기도 하였다. 규칙은 처음에는 아무런 규칙이 없었으나 동티모르 과학 교사들이 스스로 실험을 수행하도록 안내하기 위하여 실험 재료를 현지화하는 등의 규칙을 찾아 나갔다. 노동 분업은 동티모르 쪽 업무(초청, 번역, 교통, 교사 모집, 숙박, 식사, 관광 등)는 팔로모 신부가 전담하였으며 한국 교사들은 계획, 실험 선정, 실험 재료 준비, 자료집 제작, 번역, 편집, 포스터와

플랭카드 제작, 항공편 예약, 약품 준비, 봉사활동 T 셔츠 제작 등을 분담하였다. 2015 년부터 시작된 새로운 교육 방식인 ‘training of trainer’에서 일부 동티모르 교사는 과학 실험을 먼저 연수받은 후 다른 동티모르 교사에게 연수를 제공하는 역할을 담당하기도 하였다. 이상과 같이 문화역사활동이론은 봉사활동의 발달 과정을 기술하는 데 매우 유용하게 활용되었다.

(이 연구는 2015 년 대한민국 교육부와 한국연구재단의 지원을 받아 수행된 연구임 (NRF-2015S1A5A2A03048047))

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-605**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

개방형 탐구 수업을 경험한 예비과학교사의 과학의 본성 이해와 탐구 수업에 대한 인식 변화에 관한 연구

조제희 우애자[1,*]

이화여자대학교 과학교육학과 [1]이화여자대학교 과학교육과

이 연구는 예비과학교사들의 개방형 탐구 수업 경험이 과학의 본성 이해와 탐구 수업에 대한 인식에 어떠한 영향을 주는지 알아보는 것을 목적으로 하였다. 이를 위해 개방형으로 진행되는 탐구화학실험 수업을 수강하는 사범대학 과학교육과 학생들을 대상으로 수업에 대한 인식 설문 조사, 과학의 본성 이해 검사, 과학 탐구에 대한 태도 검사, 그리고 개인 면담을 실시하였다. 개방형 탐구화학실험 수업은 제시된 현상을 관찰한 후 조별로 탐구 문제를 설정하여 가설을 세우고 실험을 통해 검증하거나 자료를 수집해 탐구 문제에 대한 결론을 도출하는 방식으로 총 10 차시 진행되었다. 연구 대상은 예비과학교사 총 40 명이며, 그 중 20 명을 대상으로 추가적인 개인 면담이 이루어졌다. 이 연구의 분석 결과는 다음과 같다. 첫째, 예비과학교사들은 개방형 탐구 수업을 경험한 후 과학의 본성에 대한 이해도가 유의미하게 향상되었다(p

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-606**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

과학적·사회적 문제(Socio-Scientific Issues, SSI) 교육의 주제 선별 및 교육적 기대

박현주

조선대학교 과학교육학부

본 연구의 목적은 학생들의 과학적 소양 함양 및 SSI 교육의 학교 현장 정착을 위하여 SSI 교육 및 프로그램의 이론적 토대와 전략에 대한 기초 자료를 제공하는 것이다. 이를 위하여, 학생들의 합리적인 문제해결이나 소비자 선택을 위한 다양한 SSI 이슈들을 유목화하여 제안하여 교육과정과의 연계성을 살펴보고, 대표 주제(예를 들면, 식품첨가물, 살균제, 메탄올 사용, 불산 유출 등)에 대한 SSI 교수학습자료를 STEAM 을 적용하여 개발하여 그 효과를 조사하고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-607**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

2009 개정 과학교육과정에 따른 초등학교 과학 교과서의 읽기자료 분석

강석진

전주교육대학교 과학교육과

이 연구에서는 초등학교 과학 교과서에 제시된 읽기자료의 특성을 조사하기 위하여 2009 개정 과학교육과정에 의거하여 개발된 초등학교 과학 교과서에 제시된 읽기자료를 분석하였다. 읽기자료의 분석 기준은 주제 유형, 목적, 학생 활동, 제시 형식, 시각자료의 유형, 시각자료의 역할, 시각자료와 텍스트의 근접성 등이었다. 연구 결과, 2009 개정 과학 교과서의 읽기자료는 2007 개정 과학 교과서의 읽기자료에 비해 조금 줄어들었다. 2009 개정 과학 교과서에는 주제 유형 중 과학 지식과 실생활 응용에 해당하는 읽기자료가 많았고 첨단 과학에 해당하는 읽기자료의 개수는 조금 줄어들었다. 2009 개정 과학 교과서의 읽기자료는 제시 형식 측면에서 거의 대부분 설명식 텍스트였고, 학생 활동 측면에서는 2007 개정 과학 교과서에 비해 탐구형 읽기자료의 비율이 큰 폭으로 증가하였다. 2009 개정 과학 교과서의 읽기자료에 사용된 시각자료는 대부분 그림 및 사진이었고 본문 보조 역할의 비율이 가장 높았다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-608**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

이온 결합에 대해 고등학생이 생성한 비유의 분석: 학생의 개념이해도와 인지적 특성에 따른 특징을 중심으로

김민환 노태희*

서울대학교 화학교육과

이 연구에서는 고등학교 학생들이 이온결합에 대해 생성한 비유의 특징을 비유의 개수와 대응 관계 이해도, 비유의 소재와 유형의 측면에서 분석하고, 이 결과를 학생들의 개념 이해도와 논리적 사고력, 비유 추론 능력의 수준에 따라 비교하였다. 서울특별시에 소재한 5 개 고등학교에 재학 중인 2 학년 학생을 대상으로 2009 개정 교육과정에 의한 고등학교 화학 1 을 모두 이수한 후인 12 월말에 연구를 실시하였다.

연구 결과, 개념 이해도, 논리적 사고력, 비유 추론 능력이 높을수록 학생들은 비유를 더 많이 생성하는 것으로 나타났다. 그러나, 학생들이 생성한 비유에 대한 대응 관계 이해도는 논리적 사고력과 비유 추론 능력만 관련이 있었다. 학생들은 이온 결합에 대한 비유를 생성하기 위한 소재로 사회와 사물, 음식, 여가 등을 활용하였는데, 비유의 소재는 개념 이해도에 따라 달라졌고, 개념 이해도가 높을수록 다양한 소재를 활용하여 비유를 생성하는 것으로 나타났다. 즉, 학생들이 활용한 비유의 소재는 논리적 사고력이나 비유 추론 능력과 같은 인지적 특성보다는 개념 이해도와 더 큰 관련이 있는 것으로 나타났다. 또한, 학생들이 생성한 비유의 유형은 개념 이해도와 논리적 사고력에 따라 비유의 표현 방식이 달라지는 것과 같이 학생들의 특성에 따라 달라지는 경우도 있었으나, 상황의 작위성이나 추상도와 같이 학생들의 특성에 영향을 받지 않는 비유의 유형도 있었다. 이상의 결과를 바탕으로 교육적 함의를 논의하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-609**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

팀 별 문제 해결활동에 기반한 한국과학영재학교 일반화학 II 수업 활동 사례 발표

오진호* 천만석[1,*]

한국과학영재학교 화학생물학부 [1]한국과학영재학교 화학

6 개의 과학영재학교 또는 2 개의 과학예술영재학교 운영의 시점에서 과학영재학생들에게 어떤 그리고 어떻게 속진 및 심화교육을 제공할 것인가? 는 중요한 화두이다. 한국과학영재학교는 수학과 과학교과에서 교원의 전문성을 바탕으로 과학영재학생들에게 대학과 연계된 Advanced Placement(AP) 속진 교육 프로그램과 심화 교육 프로그램을 교육과정 안에서 운영하고 있다.화학교과목에서 대학과 연계된 AP 교과목인 일반화학 교과목을 과학영재학생들에게 어떻게 가르칠 것인가에 대해서는 지속적으로 고민을 해 오고 있는 부분이다.과학영재학교에서는 일반화학 수업은 16 명 이내의 소수의 학생들을 대상으로 분반을 개설하여 운영을 하고 있는 부분이 대학과 차별화되는 부분이다. 한국과학영재학교에서는 선택교과목으로 일반화학 1,2 그리고 일반화학실험 1,2 을 “기초유기화학”, “기초분석화학”, “분광학입문”, “나노화학의 입문” 및 “화학과 에너지” 등의 심화교과목의 선수 교과목으로 지정하여 운영하고 있다. 한국과학영재학교에서 일반화학 2 교과목을 POGIL(Process Oriented Guided Inquiry Learning) 또는 팀별 문제해결 활동에 기반한 수업을 시도 운영하고 있다.본 연구에서는 팀별 문제해결활동에 기반한 한국과학영재학교의 일반화학 2 수업 사례를 소개함으로써 과학영재학생들에게 대학의 AP 교과목인 일반화학 교과목을 어떻게 가르치는 것이 좋은 가에 대한 고민을 공유하고자 한다. 한국과학영재학교 이러한 수업의 시도는 일반화학 2 교과목에 대한 학생들의 학습뿐만 아니라, 과학영재학생들의 자기주도적인 학습능력과 팀 협동력 향상에도 도움을 줄 것으로 기대한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-610**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

중학생들의 과학 개념: 상태변화와 열에너지 개념과 연소 반응에서 질량보존 개념을 중심으로

최원호

순천대학교 화학교육과

상태 변화와 열에너지 개념과 연소 반응에서 질량보존 개념에 대하여 중학생들의 생각을 성취수준별로 조사하였다.상태 변화와 열에너지 개념을 조사하기 위해 사막을 여행하는 여행자의 양가죽 물통에서 물이 조금씩 빠져 나오면서 양가죽 물통 안의 물이 시원하게 되는 이유를 질문하였다. 학생들의 반응은 크게 물의 기화를 직접 표현하여 응답하는 유형, 물의 기화를 언급하지 않고 열의 방출이나 상태 변화로 설명하는 유형 등이 있었으며, 오개념의 경우에는 물의 열차단, 양가죽의 열차단, 온도가 높은 물질이 나가고 차가운 물질이 들어온다는 서술 등이 있었다.연소 반응에서 질량보존 개념을 조사하기 위해 강철솜을 연소시켰을 때의 질량 변화와 그 이유를 질문하였다. 학생들의 반응은 크게 산소와 결합하여 산화철을 생성한다고 표현한 유형, 공기 중 기체와 결합하거나 화학 반응을 한다고 표현한 유형 등이 있었으며, 오개념의 경우에는 결합된 물질이나 생성된 물질을 잘못아는 경우, 화학 결합 외의 설명을 하는 경우, 질량보존법칙을 잘못 적용하거나 강철솜의 질량이 변하지 않는 속성을 가져 강철솜은 연소하여도 질량이 일정하다는 생각하는 경우, 강철솜은 연소 후 기체가 빠져나가 가벼워진다고 생각하는 경우 등이 있었다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **EDEC.P-611**
발표분야: 초중등교사・화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

수소연료전지제작을 이용한 과학캠프

천만석* 오진호[1]

한국과학영재학교 화학 [1]한국과학영재학교 화학생물학부

과학캠프에서 특정 주제를 통한 경연은 학생들의 자발적인 창의력을 키우는데 많은 도움이 된다. 협동, 문제해결능력, 창의적인 생각, 특정 주제의 원리 습득과 같은 종합적인 사고를 하게한다. 또한 제작을 위한 기기의 사용 및 사용, 공학적인 사고를 할 수 있다. 2016 년 여름방학중 중학생을 대상으로 한 수소연료전지를 이용한 자동차 제작을 주제로 진행하였다. 2 명 1 조로 29 개 팀이 진행을 했으며 구입한 MEA 를 이용하여 전지를 제작하고 제작한 전지를 소형모터와 연결하여 장난감 자동차를 주어진 수소를 이용하여 멀리가는 것을 목적으로 했다. 준비된 수소연료전지의 제작 및 개량된 제작 방법, 학생들의 활동 내용 및 수소자동차 이동의 정도를 위한 방법을 소개하고자 한다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-612**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Recrystallization of insensitive high energy material

권국태 이소정[1] 김승희[2] 김진석*

국방과학연구소 4본부 2부 [1]국방과학연구소 4-2 [2]국방과학연구소 4본부2부

Sensitivity is one of the important character for the energetic materials. There were many attempts to develop high-performance and insensitive explosives. 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo [5.5.5.0.0]-dodecane is a promissing compound in the field of insensitive explosives. It has similar structural framework with HNIW(CL-20), and like it has very high density like CL-20. However this compound showed very good character in the aspect of sensitivity unlike CL-20. After synthesis of energetic compound, particle shape was controlled throgh recrystallization process. In this presentation, we will show some synthetic schemes and recrystallization result of insensitive high energy matarial.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-613**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Compartive Study of the Heat of Formation by BCA and Gaussian SW of High Nitrogen Energetic Salts of TNBI

이소정 김진석[1,*] 김승희[2] 권국태[1]

국방과학연구소 4-2 [1]국방과학연구소 4본부 2부 [2]국방과학연구소 4본부2부

TNBI(4,4`,5,5`-Tetranitro-2,2`-biimidazole)는 둔감 고성능 분자화약으로 유망한 물질이었으나, 흡습성이 높고, 이미다졸 고리의 불안정한 수소로 인한 낮은 안정성 문제점 때문에 화약으로서의 사용이 불가능하였다. 이에 TNBI 를 여러가지의 고질소염 형태로 합성하여 흡습성 문제를 해결하였고, 성능과 둔감도를 향상시켰다. 합성한 TNBI 의 고질소염은 Gaussian 프로그램을 이용하여 계산한 생성열과 Bomb calorimeter 를 이용한 실제의 생성열을 비교하였다. Explo 5 프로그램으로 폭발 성능 역시 비교 예측하였다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-614**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile electrochemical synthesis of anatase nano-architectured titanium dioxide films with reversible superhydrophilic behavior

Sorcar Saurav 인수일[1,*]

DGIST 에너지시스템공학 [1]DGIST 에너지 시스템 공학 전공

In the present work we report a facile and scalable technique for preparation of superhydrophilic Ti surfaces by electrochemical anodization having reversible wettability properties. Using a NaOH electrolyte, the electrochemically anodized Ti foils manifest nanoscale topographical features, having interconnected nanowebs and nanofibrils, that enhance surface roughness as well as light absorption. Upon 5 minute of UV illumination and warm white light illumination, a complete spreading of a 5 μL water droplet with a water contact angle (WCA) of 4.8° and 3.2° respectively, is achieved. Key factors contributing to the superhydrophilic character include surface topology and surface chemical reactions.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-615**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Fabrication of a Noble Metal-Free Photocatalyst: TiO2 Nanotube Arrays Covered with Reduced Graphene Oxide

Abdul Razzaq 인수일[1,*]

DGIST 에너지시스템공학 [1]DGIST 에너지 시스템 공학 전공

One-dimensional TiO2 nanotubes arrays (TNT) are the subject of great current interest among the photocatalysis research community, however the relatively large bandgap that provides TiO2 with its excellent charge corrosion stability severely limits its absorption of solar spectrum energy. To increase the optical absorption of TiO2 while maintaining its otherwise commendable properties a number of approaches have been investigated including doping with non-metal or noble metal co-catalysts such as platinum, coupling with low band gap semiconductors, and the synthesis of carbon-based TiO2 composites. During the past few years graphene-based TiO2 nanostructures have been found to offer improved photoelectrochemical properties, with graphene enhancing light absorption as well as promoting rapid charge transfer. With the aim of replacing expensive noble metal co-catalysts, herein we report a noble metal-free novel nanostructured photocatalytic material fabricated using a facile synthesis approach, comprising a one-dimensional array of TNT covered with a reduced graphene oxide-TiO2 nanoparticles (rGO-TiO2 NP) composite. The novel nanostructure exhibits significantly improved photocurrent density and photochemical activity via conversion of CO2 into methane under simulated solar light irradiation. The improved performance appears due to the combined effect of enhanced light absorption and effective charge separation promoted by the rGO.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-616**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

The studies of Gas permeability properties of the blended polymers composed with polynorbornene and polyimides synthesized from 6FDA-durene

유서윤 서봉국[1,*] 임충선[2]

한국화학연구원 화학산업고도화센터 [1]한국화학연구원 환경자원연구센터 [2]한국화학연구원 화학산업고도화 센터

Over the past three decades, polymeric membranes have become widely used for a variety of industrial gas separations applications due to processability and affordable costs. The hydrogen is envisioned as the optimal solution for global energy. When high concentration of hydrogen combines with oxygen, it can cause combustion or explosion. Therefore, the importance of detecting sensor for hydrogen has been augmented since hydrogen cannot be broadly used as an energy source until the sensor system for the detection of the leaked hydrogen is installed.In this study, we demonstrate the successful applications of the solution blending technique using 6FDA-durene modified polyimides and polynorbornene. The effect of variation in composition of the blended membranes upon gas permeability and selectivity was investigated. It is found that the increase of the modified 6FDA-durene in the composition resulted in the enhancement of gas permeability attributed mainly to the effect of diffusivity.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-617**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Advanced Hydrazine Solvent for Efficient CO2 Absorption

이규형 계소황[1] 허남회[*]

서강대학교 화학과 [1]서강대학교 화학

Advanced hydrazine-based solvents were developed as promising absorbents for CO2 capture. In comparison to the benchmark monoethanolamine (MEA, 30 wt %) solvent, the hydrazine-based solvents show excellent activities in terms of working capacity and absorption rate. Their overall mass transfer coefficient is about three times higher than that of MEA and their cyclic capacities are about twice larger than that of MEA. They also show the capability to capture and release CO2 for three cycles without changing their absorption capacity. These advantages could make them promising solvents for CO2 capture. On the basis of multi-nuclear NMR studies, plausible intermediates and reaction mechanism will also be presented in detail. An important finding from the NMR studies is that the absorption and desorption processes occur via the formation of two chemical species composed of hydrazine and CO2 with a 2:1 ratio.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-618**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Peroxymonosulfate Activation by the Surface-Loaded Noble Metals for Oxidative Degradation of Organic Pollutants

<u>안용윤</u>

고려대학교 건축사회환경공학부

This study explores the application of noble metals for peroxymonosulfate (PMS) activation and the associated oxidative degradation of organics. To enable the recycle of noble metal-based activators, noble metal nanoparticles were loaded uniformly on alumina and titania supports using arc plasma deposition (APD) technique. Among the tested noble metals (i.e., Pd, Pt, Au and Ag), Pd exhibited the highest capacity for PMS activation, and caused 4-chlorophenol (4-CP) oxidation that was kinetically faster at acidic pH than that when Co^{2+} was used as a common PMS activator. Pt and Au were capable of activating PMS at moderate rates whereas PMS activation was absent with Ag. In addition to the type of noble metals, PMS activation efficiency varied depending on noble metal loading and pH. The experiments to degrade various organic compounds showed that a kinetic rate of organic degradation by noble metal combined with PMS was highly substrate-specific unlike Co^{2+}/PMS. Such a distinction in reaction mechanism between noble metal/PMS versus Co^{2+}/PMS was also suggested in manifold ways: quenching effect of methanol, efficiency of methanol conversion to formaldehyde, and PMS stability in the presence of 4-CP. The results collectively imply the occurrence of the non-radical mechanism in the combined noble metal-PMS systems. Pd or Pt immobilized on alumina underwent gradual reduction in PMS activation during the repeated applications whereas the alterative use of titania as a host material improved the catalytic activity for PMS activation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-619**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cu2ZnSnS4(CZTS)-ZnO: A noble metal-free hybrid Z-scheme photocatalyst for enhanced solar-spectrum photocatalytic conversion of CO2 to CH4

Zubair Muhammad 인수일[1,*]

DGIST 에너지시스템공학 [1]DGIST 에너지 시스템 공학 전공

Development of photocatalytic materials for achieving the aspects of cost-effectiveness, improved performance and high stability is a subject of enormous interest among the photocatalysis research society. With the aim of achieving above mentioned features, we report herein a noble metal free, visible-light active, efficient and highly stable hybrid Cu2ZnSnS4 (CZTS)-ZnO photocatalyst, synthesized by a simply designed two-step process. The morphological, crystalline, optical and electronic properties of the prepared samples are intensively investigated by respective characterization techniques. The band alignment for the hybrid materials is studied using empirical calculations, which is further verified by valence band XPS measurements. Photocatalytic performance of hybrid Cu2ZnSnS4 (CZTS)-ZnO photocatalyst is evaluated by measuring, under simulated solar light, the ability of the photocatalyst to convert CO2 into hydrocarbon fuels, primarily CH4. The hybrid CZTS-ZnO photocatalyst with an optimum CZTS loading exhibits a CH4 yield of 138.90 ppm g-1 h-1, a factor of ≈ 31 times greater than the un-sensitized ZnO nanorods, and ≈ 22 times greater than the CZTS nanoparticles. Optimized sample shows excellent stability, demonstrating similar yields over five test-cycles. The enhanced performance of the hybrid, noble metal-free samples can be attributed to improved light absorption, and efficient separation of the photogenerated charge due to the Z-scheme heterojunction interface.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-620**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Aggregation and dispersion characteristics of hydrophobic nanoparticles in media: Effect of polymer

황국화 한요셉 김현중*

전북대학교 자원·에너지공학과

The aggregation and dispersion behavior of carbon black nanoparticles (CB-NPs) in ecotoxicity test media were investigated by measuring the hydrodynamic diameter and sedimentation change of CB-NPs suspension in the five types of medium during the 96hours. CB-NPs suspension was prepared by adding the CB-NPs, SRHA (suwannee river humic acid) as a representative of polymer into media. the initial concentration of CB-NPs in the media was kept as 10 mg/L and the concentration of SRHA was set up from 1 to 10 mg/L. The five types of ecotoxicity medium were selected. The ecotoxicity test media were ISO test water, Elendt M4 medium, OECD TG 201 medium (ISO 8692), AAP medium (US. EPA, ASTM), and BBM medium, which are used for the toxicity test of algae, daphnia, and fish culture. To confirm the stability properties of CB-NPs in 5 types of medium, hydrodynamic diameter and sedimentation change of the CB-NPs suspension were investigated. Significant aggregation and sedimentation of the CB-NPs dispersed in the medium were observed in 24 hours, and the stability of CB-NPs was significantly low. SRHA was added to improve the stability of the NPs in the medium, and stability tests were conducted. According to the stability test, a decreasing trend of aggregation and sedimentation between the NPs was confirmed, which was maintained in a stable dispersion status for 96 hours. To analyze the stability between the NPs, the interaction energy was calculated using the DLVO theory. the CB-NPs interaction in the medium was more accurately calculated through the extended and modified DLVO theories rather than through the classical DLVO theory.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-621**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on Thermal Property by DSC&ARC with different AP Quality

김승희* 권국태[1] 이소정[2] 김진석[1]

국방과학연구소 4본부2부 [1]국방과학연구소 4본부 2부 [2]국방과학연구소 4-2

AP(Ammonium Perchlorate, NH_4ClO_4)를 포함하는 복합화약조성의 등온가열시험(ISCO) 시, 일정 등급 이하의 AP 를 사용하는 경우 "Bulged"현상으로 인해 정상적인 등온가열시험 결과를 얻을 수 없었다. 본 연구는 고품질의 AP 와 저품질의 AP 의 열적 안정성 차이를 규명하기 위해 모든 LOT 의 AP 에 대해 일반 DSC 결과 및 고압팬을 이용한 DSC 결과, 또한 ARC(Accelerating rate calorimeter) 결과와 비교분석하여 그 경향성에 대해 분석하고, 고압팬을 이용한 열분석 결과로 AP 품질을 규격화하였다.

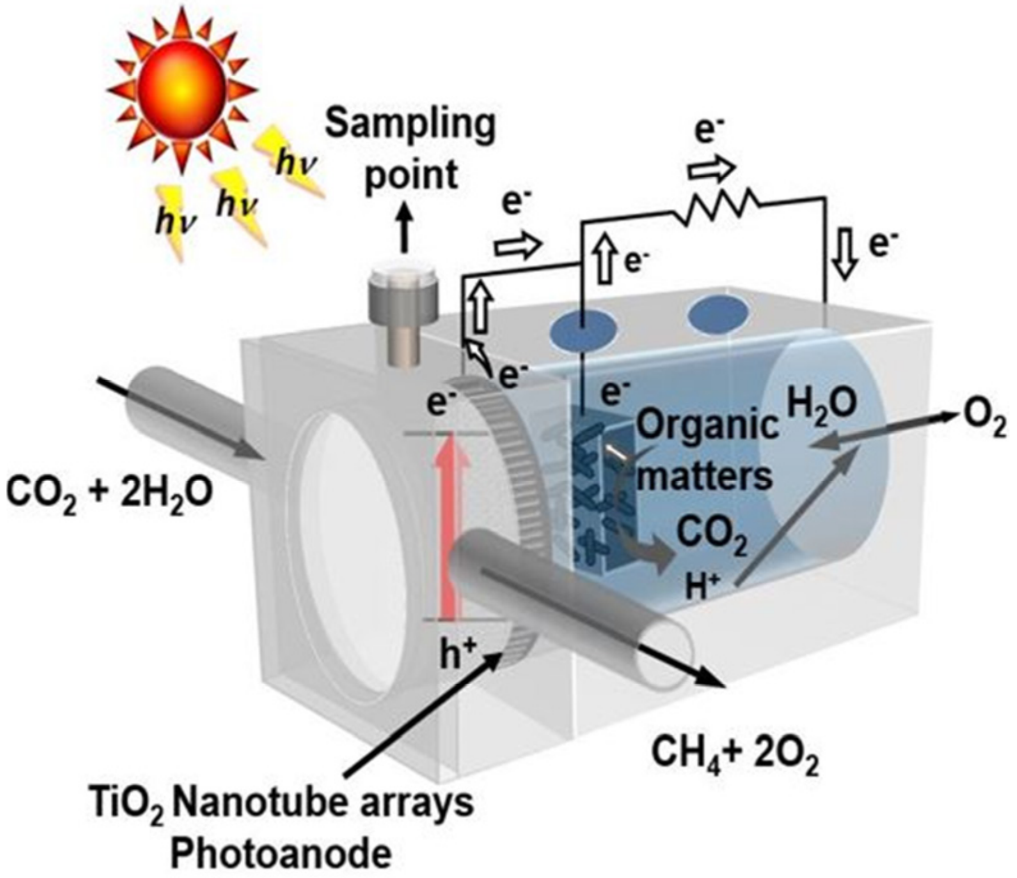
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-622**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photo- coupled Bio-Anode: A New Approach for Improved Microbial Fuel Cell Performance

이경석 이승현 인수일[1,*]

DGIST 에너지시스템공학전공 [1]DGIST 에너지 시스템 공학 전공

Microbial fuel cells (MFCs) offer a promising opportunity for harvesting energy from wastewater, however energy densities are still relatively low limited, in part, by a kinetically slow oxygen reduction reaction. Herein we present an innovative approach to enhance MFC power output by pairing a TiO2 nanotube arrays (TNT) photoanode with the bioanode of a normal MFC. Unlike various approaches of air cathode modification, the focus of the present work is to synergistically couple photo- and bio- anodes, moderating oxygen reduction reaction limitations to thereby increase output power density. From our hybrid-MFC we achieve a power density of 1284 ± 20 mW/m2 and a current density of 7142.9 mA/m2, values approximately 1.5 and 1.9 times higher, respectively, than a normal MFC. Further, using the TNT photoanode we demonstrate CO2 photoreduction, suggesting the simultaneous use of the hybrid-MFC for power generation and reduction of atmospheric CO2 concentrations.


hν
hν
hν
Sampling point
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
e⁻
$CO_2 + 2H_2O$
Organic matters
H_2O
O_2
CO_2
H^+
h^+
$CH_4 + 2O_2$
TiO_2 Nanotube arrays Photoanode

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-623**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Evaluation of Carbon Dioxide Efficiency in Flue Gas of Magnesium Oxide-doped Carbon Adsorbents synthesized by Microwave-Assisted Method

허영정 박수진*

인하대학교 화학과

In this study, magnesium oxide (MgO)-modified carbon materials were fabricated using $Mg(NO_3)_2$ and microwave-assisted irradiation The properties and textural structures of the prepared materials were characterized using powder X-ray diffraction, elemental analysis, and N_2 adsorption/desorption experiments. The X-ray diffraction patterns showed the characteristic diffraction peaks of MgO at 43° and 62.5°, and no impurities were apparent. By changing the microwave reaction time, the spherical structure of the parent material was transformed to a hybrid structure with MgO crystalline particles in a carbon matrix. The morphology evolution and properties of the prepared materials were also investigated using transmission electron microscopy and N_2 adsorption, respectively. The CO_2 adsorption performances were also investigated, through isobar experiments under a mixed gas flow (15% CO_2 in N_2). It was found that MgO affected the CO_2 capture behavior by enhancing the fundamental characteristics of the carbon surfaces

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-624**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of H_2O_2/Steam Activation on Porosity and Surface Characteristics of Activated Carbons for CO_2 Capture and CO_2/N_2 Selectivity

허영정 박수진[*]

인하대학교 화학과

Ultramicroporous carbons were prepared from starch by physical activation with oxidant at different temperatures. A significant proportion of the porosity in the carbons is contributed by micropores. Physical activation using steam was observed to have an influence on the development of new pores and the expansion of pore sizes and to be effective in developing optimal micropores for CO_2 adsorption on the carbon surface. This resulted in porous carbons with enhanced CO_2 adsorption capacities and CO_2/N_2 separation abilities without chemical activation.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-625**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

PVA-assisted combustion synthesis of KNO_3-MgO absorbent for CO_2 capture at intermediate temperature

오경렬 곽진수 김강영 권영욱*

성균관대학교 화학과

Carbon capture and storage (CCS) is one of the most promising technologies that can mitigate global CO_2 emissions. Alkali metal nitrate promoted MgO absorbents are well known for CO_2 capture at intermediate temperature (200-500℃). In this study, KNO_3 promoted MgO absorbent was synthesized by combustion method assisted with polyvinyl alcohol (PVA) and its CO_2 capture properties were analyzed. PVA was dissolved in addition to KNO_3 and $Mg(NO_3)_2$ in water as a complexing agent for metal cations and burnt to ashes by torch after drying process. Following calcination process removed carbon sources entirely, only MgO and potassium species was remained. This synthesis includes coordination between hydroxyl group of PVA and metal cations, which derives interesting reaction kinetics for CO_2 absorption. Temperature swing absorption (TSA) shows that this absorbent has several reaction steps as temperature increases under CO_2 condition and this trend was observed in isothermal CO_2 absorption test as well. CO_2 absorption properties of the absorbent were further studied by cycle test.

대한화학회 제118회 총회 및 학술발표회 (The 118th General Meeting of the Korean Chemical Society)

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-626**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Proton Conductivity in a Graphene/Nafion Composite Membrane

Benjamin Cunning Thomas Bayer[1] Stephen M Lyth[1] Rodney Scott Ruoff[2,*]

기초과학연구원 다차원탄소재료연구단 [1]I2CNER, Kyushu University [2]UNIST 화학과

Proton exchange membrane (PEM) fuel cells ideally operate at high temperatures. Above 100 °C the kinetics of the oxygen reduction reaction are much higher, tolerance to fuel impurities are improved and water and heat management are simplified[1].Graphene, a single layer of sp2 hybridized carbon has been shown to be stable in oxidizing environments up to 200 °C[2], impermeable to hydrogen[3], and more recently, allow proton transport through the plane[4]. These properties make graphene an ideal material in a PEM fuel cell.Here we demonstrate a composite graphene PEM based on a single layer of graphene sandwiched between two thin layers of Nafion. At elevated temperatures and humidities, the graphene/Nafion composite was found to possess through plane proton conductivities similar to pure Nafion. We also demonstrate the composite material has good gas barrier properties compared to pure Nafion films.*This work was partly supported by IBS-R019- D1.*[1] A. Chandan et. al., J. Power Sources, 2013, 231, pp264[2] S.Chen et.al., ACS Nano, 2011, 5, pp1321[3] J. Scott Bunch et. al., Nano Lett., 2008, 8, pp2458[4] S. Hu et. al., Nature, 2014, 516, pp227

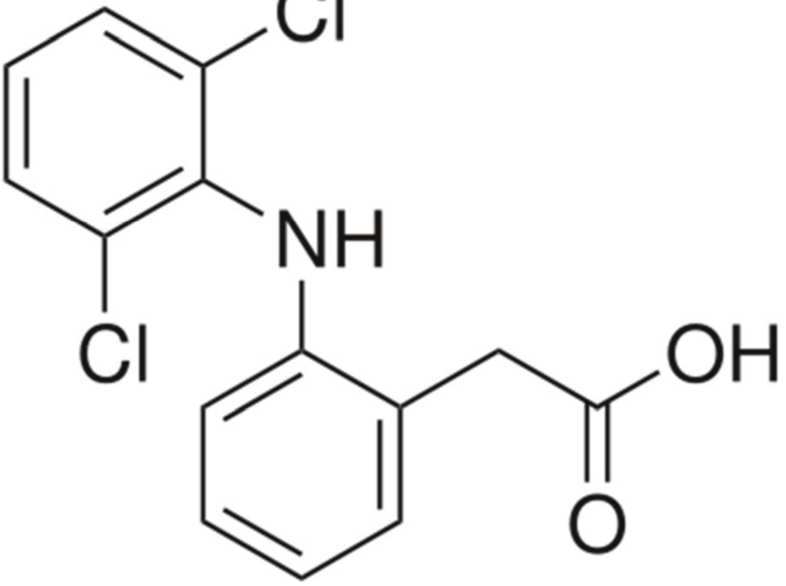
일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-627**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

환경에 유입된 난분해성 의약품(diclofenac)의 친환경적 제거 연구

김동욱

육군사관학교 화학과

의약품의 사용이 급증하면서 사람의 대사에 의해 분해되지 않는 약품들이 인간의 배설물 등에 의해 자연으로 배출되면서 소량의 약품들이 자연 및 폐수에 발견되는 경우가 점점 증가하고 있다. Diclofenac 은 진통소염제의 일종으로 하수처리장 배출수 또는 자연수에서 발견이 되는 흔한 약품 중 하나이다. 낮은 수준의 농도라도 칵테일효과에 의해 자연생태계에 큰 영향을 끼칠 수 있음이 알려져 있으므로 이러한 약품이 자연에 배출되지 않도록 하수처리 과정을 거쳐 제거할 필요성이 제기되고 있다. Diclofenac 의 친환경적 제거에 대한 연구가 활발하게 진행이 되고 있다. 특히 오존(O_3), 오존과 과산화수소(O_3 and H_2O_2), 자외선(UV), 광펜톤 반응 등을 활용한 고도처리기법(Advanced Oxidation Process, AOP)이 집중 연구되고 있다. 본 연구는 세종과학고등학교의 R&E 과제의 일환으로 수행된 연구이다. 본 연구에서는 팔라듐산화물(palladium oxide), 영가마그네슘(zero valent Mg), 영가철(zero valent iron)등의 heterogeneous phase 물질을 활용하여 diclofenac 을 제거하고자 한다. 위에 언급된 물질들은 수용액 상에서 쉽게 혼합이 되며, 반응성이 좋을 뿐 아니라 반응 후 필터를 통해 쉽게 회수 또는 제거할 수 있을 뿐 아니라 부산물이 친환경적인 산화물이므로 친환경적인 대안이 될 수 있다. 세가지 물질을 활용한 diclofenac 의 친환경적 제거를 탐구한다.


Cl
NH
Cl
OH
O

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-628**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

국내 과불화옥탄산(PFOA)의 현황 및 노출 위해성 연구

박지홍 이승규[1,*]

to21 위해성연구 [1](주)티오이십일 위해성연구팀

전세계적으로 잔류성유기오염물질("POPs")로 인해 환경 및 인체의 유·위해성에 대한 우려가 높아짐에 따라 국제기구 및 주요 선진국을 중심으로 대상 물질에 대한 국제적 사용 및 유통을 금지하기 위한 다양한 노력들이 진행되고 있다. 우리나라도 이러한 국제 사회의 움직임에 대응하기 위해 이들 대상 물질에 대한 각 매체별 배출저감 연구방안 및 조사를 꾸준히 진행하고 있다. 최근 전 세계적으로 유해성에 대한 논란이 끊임없이 제기되고 있는 물질이 과불화합물의 일종인 PFOA(perfluorooctannic acid)이다. PFOA 는 현대 사회에서 필수적인 물질로써 지난 50 년간 수많은 산업현장에서 사용되고 있으나 최근 잔류성, 발암성 등 독성에 대한 우려가 높아짐에 따라 스톡홀름 협약 상 등재 후보물질로 지정되어 있다. PFOA 는 다른 잔류성 물질들과는 다르게 후라이팬, 아웃도어 등 실생활에서 쉽게 접할 수 있는 제품에 많이 사용되고 있는 물질로 국내에서도 인체 노출에 대한 논란이 제기되고 있다. 동물 실험을 통해 발암성 및 독성이 높은 물질로 평가되어 있으나 일부 연구자들에 의해 생활용품을 통한 인체노출은 매우 미미한 수준이라는 결과가 제시 되어 있으며, EU, 미국 등 주요 선진국에서는 PFOA 사용지침 마련을 위한 연구가 이미 진행되고 있다. 우리나라는 이들 국가에 비해 제품을 사용하는 빈도 및 함유 농도가 낮게 유지되고 있고, 식약처에서 발표한 연구보고서에서는 후라이팬 등 주요 함유제품 사용으로 인한 검출량이 매우 미미한 수준으로 나타났다. 하지만 PFOA 는 반감기가 매우 길고 생물 축적성이 강하기 때문에 향후 국민들의 건강 및 안전성 확보를 위해 관리체계 확립 및 규제방안 마련을 위한 노력이 필요하다.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-629**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Influence of Microposority and Surface Characteristics on CO$_2$ Capture and CO$_2$/N$_2$ Selectiviety of PAN/PVDF Composites based Porous Carbons

<u>허영정</u> 박수진*

인하대학교 화학과

Recently, public awareness of the global climate change crisis has increased and methods to reduce emissions of greenhouse gases such as carbon dioxide (CO$_2$) are being intensively researched. Several strategies for reducing CO$_2$ emissions have been proposed, and studies have been directed toward CO$_2$ capture and sequestration (CCS). A number of separation technologies could be applied with post-combustion step. These include adsorption, absorption, membranes, and cryogenics Adsorption method uses porous solid CO$_2$ adsorbents such as zeolites, porous silicas, metal organic frameworks (MOFs), and porous carbons. These adsorbents are regenerated by temperature swing adsorption (TSA) or pressure swing adsorption (PSA). In this work, we have prepared PAN/PVDF composites via electrospinning. And then, the carbonization and activation process were performed to obtain the porous carbons for CO$_2$ capture. The features and morphologies were observed by SEM and TEM measurements. The microcrystalline characteristics were measured by XRD, and the surface properties were investigated by XPS. The textural properties were analyzed by N2/77 K adsorption/desorption isotherms. The CO$_2$ adsorption capacities were measured at 298 K. 15% CO$_2$ adsorption capacities were measured by TGA method at specific condition. These results demonstrate the successful fabrication of porous carbons with enhanced CO$_2$ adsorption capacities. Our results indicate that porous carbons are promising adsorbents for CO$_2$ capture.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-630**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation and characterization of porous carbons derived from wood pellet for hydrogen storage

한예지 박수진[1,*]

인하대학교 화학화학공학융합대학원/화학 [1]인하대학교 화학과

In recently, the energy shortage was caused by limited energy resources and serious environmental calamities. Therefore, there is a need for finding new and efficient sources of energy. Among them, hydrogen has been perceived as an ideal and suitable energy source, owing to its renewable and clean energy characteristics. To use hydrogen as an energy source, the adsorption of hydrogen in porous materials is suitable for hydrogen storage, due to the reversibility and stability of the method, which is crucial for suitably utilizing hydrogen energy. In this work, porous carbons were prepared as adsorbents for hydrogen storage. The wood pellet (WP) was carbonized at various temperature and then used as adsorbents. The structural and morphological properties were investigated by X-ray diffraction (XRD) and scanning electron microscope (SEM), respectively. The specific surface area and micropore size distribution were investigated by N_2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and Horvath–Kawazoe (HK) method. The hydrogen storage capacities were analyzed at 77 K and 1 bar. From the results, it was found that the hydrogen storage behaviors were influenced by specific surface area, pore size, and micropore volume of the prepared samples.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-631**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of activated ketjgenblack and their hydrogen storage capacity

한예지 박수진[1,*]

인하대학교 화학화학공학융합대학원/화학 [1]인하대학교 화학과

In this work, the porous carbons were prepared as adsorbents for hydrogen storage. Among carbon black, kejtenblack (KB) was used as carbon adsorbents and was chemically activated by KOH. The structural and morphological properties were analyzed by X-ray diffraction (XRD) and scanning electron microscope (SEM), respectively. The specific surface area and micropore volume were investigated by $N_2$2/77 K adsorption isotherms using Brunauer-Emmett-Teller (BET) equation and Dubinin-Radushkevic (D-R) equation. The hydrogen storage capacities were analyzed at 77 K and 1 bar. From the results, it was found that the hydrogen storage capacities were influenced by KOH activation that increases specific surface area and micropore volume of the prepared samples.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-632**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Improving the Water Stability of Hybrid Polymer-MOF by Photo Polymerization for Emerging Contaminants Adsorption

최정아 김진오[1] 김동표[*]

POSTECH 화학공학과 [1]POSTECH 미세유체응용화학연구단/화학공학과

We have achieved the integration of hydrophobic HKUST-1@PFPE particles with high MOFs content (≈ 90 wt %). This hybrid MOFs prepared for removal of water contaminants, as well as the effect of water stability on the performance of the fluoropolymer coated MOFs. We find that the contaminants removal performance of HKUST-1@PFPE is unprecedented, with greatly improved stabilization of MOF toward both humidity and contaminants, when compare with HKUST-1powder.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-633**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cultivation of microalgae species in mixed wastewater for biodiesel and useful substance

김영석 박영태[1] 김태정[1] 함정엽[1,*]

강릉원주대학교 화학신소재학과 [1]한국과학기술연구원(KIST) 천연물연구소

Effect of wastewater, pretreated manure and acid mine drainage, on the produce lipid and ß-carotene of green micro algae, *Uronema sp.* KGE 3 and *Acutodesmus obliquus* KGE 25, cultivated in two types of wastewaters was investigated. Different dilutions (1/1-1/19) of wastewater with distilled water and wastewater were tested at atmospheric condition. *Uronema sp.* KGE 3 showed the highest growth (0.51±0.03 g L-1) with 4th culture medium (P.M.: AMD = 1: 9) and lipid content (52 % dry weight biomass) with 6th culture medium (P.M.: AMD = 1:19). *Acutodesmus obliquus* KGE 25 showed the highest ß-carotene productivity (7.4 mg L-1). The 10 mg·L-1 iron suitable amount of cell growth increasing but more than 50 mg·L-1 iron could be inhibit the cell growth. When the concentrations of ammonium were over 10 mg·L-1, the cell growth were decreased. The more concentration iron and ammonium added, the more lipid and ß-carotene was produced. Application of pretreated manure and acid mine drainage wastewaters improved the growth, lipid/carotenoids productivity and nutrient removal efficiency of *Uronema sp.* KGE 3 and *Acutodesmus obliquus* KGE 25, which can be a cost effective strategy for microalgal biomass production. Moreover, the microalgae extracts were tested for determine the possibility of the anti-cancer effect.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-634**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Freezing effect on bromate reduction by organic compounds

민대위 최원용[1,*]

POSTECH 환경공학과 [1]POSTECH 환경공학부

A significant amount of bromate might be produced as a disinfection by-product (DBP) and introduced into the aquatic ecosystem as a result of the wide-spread use of ozonation for water treatment. Understanding the fate of this toxic species in nature becomes highly important to evaluate the potential impact of bromate. In this work, the reduction reaction of bromate was studied in ice phase. The results showed that the reduction of bromate is significantly enhanced in ice especially in the presence of humic substances (humic and fulvic acids) and other organic electron donors having carboxyl, hydroxyl, and aldehyde functional groups. This reduction process produced hypobromite and bromide as the final product. However, the bromate reduction in the aqueous phase was negligible. This observed enhancement of bromate reduction in the ice phase is likely due to the freeze concentration of bromates and various electron donors in liquid-like ice grain boundary region. The present results demonstrated the vital role of humic substances and other organic electron donors towards the reduction of bromate in icy environment. These results provide evidence that the freeze-thaw cycle of nature would help transform carcinogenic bromate into less toxic species like bromide and this proposed process might be important in the polar environment.

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-635**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Vacuum Process Based Dry Transfer of Active Layer for PTB7:$PC_{71}BM$ Organic Photovoltaic Devices

이종화 김강민 장웅식[1] 안선용[1] 김영윤 박오옥[*] 왕동환[1,*]

KAIST 생명화학공학과 [1]중앙대학교 창의ICT공과대학 융합공학부

Recently, stamping transfer technique, which is considered as an alternative to spin coating process, have been actively researched to be used in organic solar cell due to intermixing problem of spin coating. Furthermore, many advantages of stamping transfer technique were reported in many recent studies such as simple and repeatable process suitable to large area fabrication, low-cost and flexibility. Nonetheless, the power conversion efficiency (PCE) of those devices in previous researches remained low performance around 4% of PCE not enough to commercialization. In this work, to overcome efficiency limit in previous reported organic solar cell fabricated by stamping transfer, we fabricated poly({4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b′]dithiophene-2,6-diyl}{3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl}) : [6,6]-phenyl-C71-butyric acid methyl ester (PTB7:$PC_{71}BM$) based solar cells via stamping transfer with polyurethane acrylate (PUA) stamp. With optimized surface energy of the PUA stamp, the bulk hetero junction (BHJ) layer was completely transferred onto poly-(3,4-ethylenedioxythiophene):poly (styrenesulfonate) (PEDOT:PSS) layer. An additional vacuum treatment was needed to transfer BHJ layer successfully due to 1,8-diiodooctane (DIO) co-solvent. As a result, stamping transferred BHJ devices have shown comparable PCE (7.11%) with those made by spin coating process (7.29%). Specially, we discovered significantly improved long-term stability of device performance in the PTB7:$PC_{71}BM$ based solar cells fabricated by stamping transfer

일시: 2016년 10월 12~14일(수~금) 3일간
장소: 부산 BEXCO
발표코드: **ENVR.P-636**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Thermal and Structural Properties of Liquid Crystal Emulsion Containing high Ceramide

노민주

코스맥스(주) 이노베이션랩

피부 각질층의 세포간지질은 주변 환경으로부터 피부를 보호하고, 표피의 수분 증발을 막아주는 등 피부 장벽 기능에 중요한 역할을 한다. 이러한 피부 각질층은 세포간지질인 세라마이드, 콜레스테롤, 지방산 등으로 구성되어 있으며, 멀티 라멜라 구조를 이루고 있다고 알려져 있다. 본 연구에서는 피부 각질층의 구조를 모사하고, 세포간지질 중 50% 이상을 구성하는 세라마이드를 고함유한 액정에멀젼을 제조하였다. 제조한 액정에멀젼은 시차주사 열 측정법(DSC), 경도 측정으로 안정성을 확인하였고, 편광현미경(POM), X 선 소각 및 광각 산란(SAXS, WAXS) 측정을 통해 멀티 라멜라 액정 구조임을 확인하였다.