대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **INTL-1**
발표분야: 기조강연
발표종류: 기조강연, 발표일시: 목 16:00, 좌장: 남좌민

Chemical Biology in Translation

Carolyn R. Bertozzi

Stanford University and Howard Hughes Medical Institute

Research at the interface of chemistry and biology has brought forth numerous technologies for modulating biological pathways and engineering biomolecules with new functions. Over the past two decades, several technologies that merge chemical and biological processes have matured to the point of clinical translation. This presentation will highlight work from our lab that aligns with this theme.

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발표분야: 기념강연
발표종류: 기념강연, 발표일시: 금 11:00, 좌장: 박진균

Microfluidics: Future Synthetic Tools

김동표

POSTECH 화학공학과

Microfluidic reactors manipulate fluids in the confined space on a scale of hundreds micrometres. Continuous-flow microreaction technology is attractive owing to inherent advantages such as efficient heat transfer and rapid mixing. It enables greater control of reaction conditions and safe operation in small volume usage, easy up-scaling, and the integrated operation. In here, various microreactors and their applications will be presented as new and future platforms for synthetic chemistry. These systems and techniques are used to carry out novel syntheses that are not or less feasible by conventional tools and process, which gets progressively incorporated into mainstream of chemistry.

•Microfluidic systems

The reactor requires resistant materials to temperatures, organic solvents, and needs efficient design for high mixing efficiency. Typically, polyimide (PI) film microreactor was fabricated by lamination of the patterned multiple numbers of films, up to 7 sheets, and a simple one-step multilayer bonding process. The multiplayered PI reactor provided 3D serpentine microchannel structure with chemically inert toward organolithium reagents and also robust to several hours of exposure to liquid N_2 and high pressures. This chip microreactor could deliver a reaction time in the submillisecond range for outpacing rapid intramolecular rearrangements, anionic Fries rearrangement. In addition, the synthesis of afesal with anthelmintic activity demonstrated its potential for practical synthesis and production.

•Continuous-flow and integrated process

Multiphase processes involving gas–liquid–solid offers clear advantages over conventional methods due to the increased surface-area-to-volume ratios, efficient mixing of reagents leads to improve reaction yields and/or selectivities. A serial process of chemical synthesis, its purification and utilization for a desired synthesis was conducted. In particular, microseparations via liquid-gas distillation in the binary phase of laminar flow to purify the generated reagents were demonstrated by fabricating the microreactor embedded with Si nanowired superamphiphobic structured channel.

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발표분야: Recent Trends in Polymer Synthesis: Controlled Molecular Weights, Morphology, and Beyond
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 김정곤

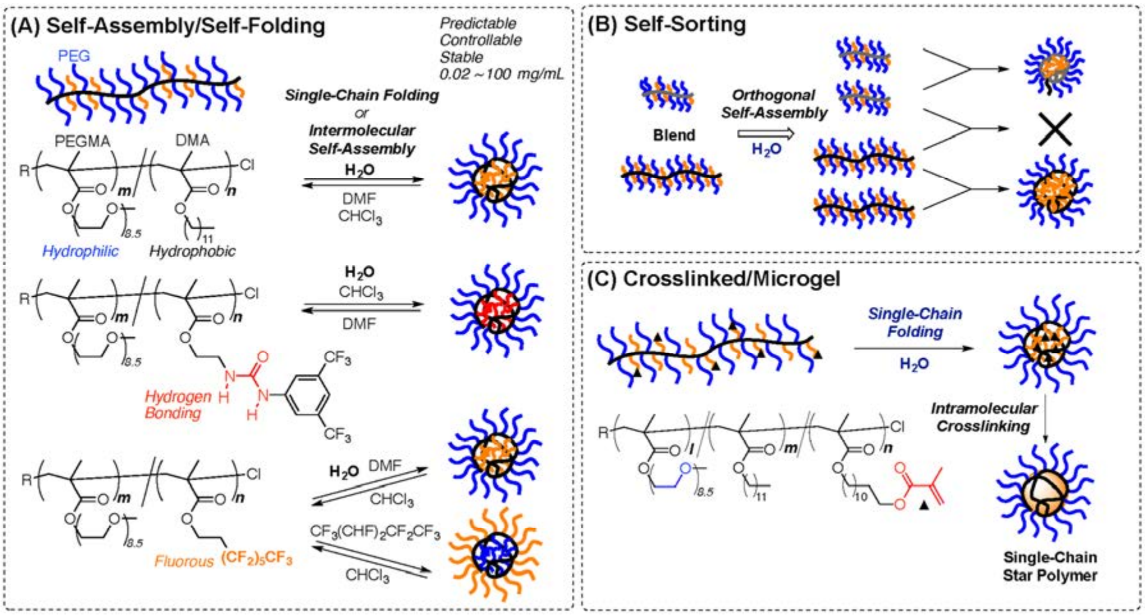
Self-Assembly and Self-Sorting of Amphiphilic Random Copolymers: From Design to Functions

Takaya Terashima

Department of Polymer Chemistry, Graduate School of Engineering, Kyoto University, JAPAN

In this paper, we report the recent advances on precision synthesis, self-assembly, and functions of amphiphilic random copolymers. PEGMA/RMA amphiphilic random copolymers, prepared by living radical copolymerization, formed self-folding polymers in aqueous or organic media. The folding properties were controlled by selecting co-monomers (RMA: hydrophobic DMA, hydrogen-bonding, fluorous) and tuning primary structure (molecular weight, composition).[1-4] PEGMA/DMA random copolymers further afforded precision "intermolecular" self-assembly into uniform nanoparticles in water, where the size, molecular weight, and aggregation number were predictably controlled.[5] In binary blend, PEGMA/DMA random copolymers with different DMA composition induced self-sorting in water to give discrete nanocompartments with different DMA composition.[5] Additionally, self-folding amphiphilic random copolymers in water allowed selective intramolecular patching into single-chain crosslinked star polymers with designer cores.[6]

References 1) Terashima, T. *Polymer. J.* **2014**, *46*, 664. 2) Terashima, T.; Sugita, T.; Fukae, K.; Sawamoto, M. *Macromolecules* **2014**, *47*, 589. 3) Koda, Y.; Terashima, T.; Sawamoto, M. *Macromolecules* **2016**, *49*, 4534. 4) Matsumoto, K.; Terashima, T.; Sugita, T.; Takenaka, M.; Sawamoto, M. *Macromolecules* **2016**, *49*, 7917. 5) Hirai, Y.; Terashima, T.; Takenaka, M.; Sawamoto, M. *Macromolecules* **2016**, *49*, 5084. 6) Terashima, T.; Sugita, T.; Sawamoto, M. *Polym. J.* **2015**, *47*, 667.


(A) Self-Assembly/Self-Folding
Predictable
Controllable
Stable
0.02 ~ 100 mg/mL
PEG
Single-Chain Folding
or
Intermolecular
Self-Assembly
H_2O
DMF
$CHCl_3$
PEGMA
DMA
R
Cl
m
n
8.5
11
Hydrophilic
Hydrophobic
H_2O
$CHCl_3$
DMF
CF_3
Hydrogen
Bonding
CF_3
H_2O
DMF
$CHCl_3$
$CF_3(CHF)_2CF_2CF_3$
$CHCl_3$
Fluorous
$(CF_2)_5CF_3$
(B) Self-Sorting
Blend
Orthogonal
Self-Assembly
H_2O
(C) Crosslinked/Microgel
Single-Chain
Folding
H_2O
Intramolecular
Crosslinking
l
m
n
8.5
11
10
Single-Chain
Star Polymer

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Synthesis and Characterization of Well-defined P3HT based Self-assembled Nanomaterials

백경열

한국과학기술연구원(KIST) 물질구조제어연구센터

Two series of well-defined poly(3-hexylthiophene) (P3HT) based self-assembled nanomaterials were prepared by the interaction of functionalized P3HTs and nanomaterials. As the first series, P3HT star polymers with gold nanoparticle (NP) core were synthesized by ligand exchange reaction between linear end-functionalized P3HT (P3HT-SH) and gold NP in solution. Obtained P3HT star polymers with gold NP core showed extremely high molecular weights (Mw ~ 3,000,000) and were well-dispersed both in solution and in solid, which was interestingly not crystallized because of unique 3-dimenstional structure. Second series of P3HT based self-assembled nanomaterials was prepared by the reaction of P3HT based block copolymer and carbon nanotube (CNT) through pi-pi interactions, where the other block copolymer, poly(neopentyl sulfonated styrene) (PNSS) was grafted to P3HT wrapped CNT. This grafted PNSS was then directly converted sulfonic polystyrene (SPS) by in-situ heat processing in solid state, which effectively doped the surface of P3HT on CNT to improve the conductivity.

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Development of wide bandgap polymers containing weak accepting moieties for efficient organic photodetectors

정인환* 윤성철[1] 이창진[2]

국민대학교 응용화학과 [1]한국화학연구원 화학소재연구단 [2]한국화학연구원 연구기획조정본부

The photoelectric effect is that light is converted into an electric current, similar to eyes, and the most popular photoelectric devices are CMOS image sensors and digital X-ray sensors. For their flexible application, we have developed several conjugated polymers containing weak electron accepting moieties to absorb the green-yellow light effectively. We modified the π conjugation length of the polymer backbone to promote the molecular stacking and the charge transfer process. In addition, the different molecular orientation of polymer chains gave a significant effect on photo-sensitivity and photo-detectivity, resulting in the promising detectivity of over 10^{13} Jones up to -2V. UV-vis spectra, space-charge limited current (SCLC) mobility, two dimensional grazing incidence X-ray diffraction (2D-GIXD) patterns, and transmission electron microscopy (TEM) were investigated, in detail, to support the our expectations and photoelectric properties.

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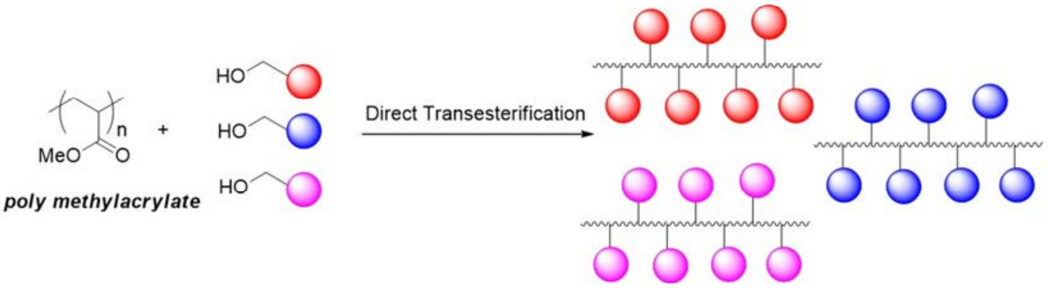
발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: 송창식

Synthesis of Functional Polyacrylate Libraries – Direct Transesterification of Polymethylacrylate

김정곤

전북대학교 화학과

Functional polymers with well-defined architectures, molecular weight distribution, and precise location of the functional groups are of utmost importance in modern polymer research and neighboring disciplines. Despite the versatility and amplified tolerance to most functional monomers, living/controlled polymerization techniques suffer from difficulties when it comes to creating a library of functional polymers with identical degree of polymerization and functional group distribution, highly essential for their structure-property relationship studies.In this regard, post-polymerization modification offers a beneficial alternative approach for tailoring multifunctional macromolecules by introducing the dissenting functional group after the polymerization step. However, it requires a highly efficient chemical reaction on a polymer chain to ensure near quantitative installation of functional units. As many chemical reactions have been introduced for post-polymerization modifications, many of them begin with polymer chain containing reactive site. The sequence of functional monomer synthesis, polymerization, and functionality transformation is a general approach. If we could directly install functional groups into a commodity polymer, it would ultimately desirable. Our research group is recently investigating a direct transesterification of poly methylacrylate with a range of alcohols of interesting structures. The development of reaction system and its current status will be presented.


MeO
O
n
+
HO
HO
HO
poly methylacrylate
Direct Transesterification

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In Situ Nanoparticlization of Conjugated Polymers

최태림

서울대학교 화학부

In some cases, the single polymer chain itself exhibits the nanostructures while others do so via self-assembly process. In this presentation, we will focus on the formation of nanostructures via the self-assembly approach. We will introduce a new concept of self-assembly termed “in situ nano-particlization of conjugated polymers”. This method produce supramolecules directly during the polymerization and no further post-modification is required. These polymers are characterized by UV-vis, IR, AFM, TEM, and DLS to obtain the detailed structural information. Here, we will show two reactions, ROMP of cyclooctatetraene and GRIM polymerization of various aromatic monomers and discuss how various nanostructures are formed in each cases.. Lastly, we will finish this talk by introducing very simple one-shot polymerization to achieve INCP and this greatly simplifies the process getting to nanostructures.

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발표코드: **POLY2-1**
발표분야: [English Session - IBS 심포지엄] New Directions in Polymer Science (※IBS 첨단연성물질 연구단 공동개최)
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: Janet Wong

Studying the Dynamics of Complex Coacervates with Super-Resolved Microscopy

John King[*] **Anisha Shakya**[1]

기초과학연구원 (IBS) 첨단연성물질연구단 [1]*기초과학연구원 첨단연성물질연구단*

Solutions comprised of oppositely charged polyelectrolytes assemble into liquid-liquid phase separated coacervates. The practical function, often exploited by living cells, is to isolate, concentrate and protect components of the cell without the use of membranes. To carry out these vital functions, coacervates must remain highly dynamic and avoid aggregation and entanglement of the components. Here, we study the dynamics of in vitro polymer-ATP and polymer-ATP-DNA coacervates using a combination of super-resolved fluorescence microscopy and fluorescence correlation spectroscopy (FCS). This experimental approach allows the diffusion of the comprising species to be studied as a function of length scale, ranging from 200 nm (diffraction limited) to 60 nm. We find a strong dependence of the local diffusion on the measurement length scale, which is not consistent with simple Brownian diffusion.

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발표코드: **POLY2-2**

발표분야: [English Session - IBS 심포지엄] New Directions in Polymer Science (※IBS 첨단연성물질 연구단 공동개최)

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: Janet Wong

Teasing Bio-inspired Micro-Reactor Chemistry out of Simple Polymer Solutions

WANG HUAN GRANICK STEVE[1,*]

기초과학연구원 천단연성물질연구단 [1]기초과학연구원 첨단연성물질연구단

We live in an age where research fields benefit from cross-pollination. In living cells, liquid droplets, which mostly are dynamical assemblies of macromolecules, function to enable chemical reactions by concentrating reactants through this nonequilibrium process. We have noticed that droplets of polymer in volatile solvent similarly concentrate into local dynamical pockets as evaporation proceeds. This presents interesting new physics on the one hand as the influence of polymer viscoelasticity in this nonequilibrium situation is subtle. It also presents chemists with a practical tool to trigger chemical reactions that in the bulk solutions would at equilibrium not occur or cease reaction by selective depletion of reactants into pockets.

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발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: Janet Wong

Watching entangled DNA with different topologies in real time with super-resolution

지아영 **GRANICK STEVE***

기초과학연구원 첨단연성물질연구단

In this talk, we will show how we unraveled the conformational dynamics of entangled linear, branched, and ring-shaped polymers in network, which is one of the most well-known problems in polymer physics, using deep imaging based on super-resolution fluorescence imaging, stimulated emission depletion (STED) microscopy. By using home-written software, we obtained the statistics of each of the hundreds of molecules, mapping out a large statistical distribution. Through inspection we not only found some aspects of the classic understanding of polymers, but some surprising aspects as well.

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발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: Janet Wong

Extreme Mechanics of Polymer Vesicles

장현숙 **GRANICK STEVE***

기초과학연구원 첨단연성물질연구단

We introduce the concept of using polymer vesicles (``polymersomes") as a platform to understand the extreme mechanics of viscoelastic closed membranes. Controlling the stress by adjusting osmotic imbalance between inside and outside these shapes, controlling the strain rate by adjusting the rate at which osmotic imbalance is applied, and controlling the viscoelasticity by varying the molecular weight and degree of entanglement, our direct optical imaging by in situ bright microscopy reveals stretching, rupturing, buckling and fingering. These distinctly different deformation patterns are also influenced by toughening the membranes to form 2D nanocomposite, for example using CdS quantum dots. Whereas applications of polymersomes to encapsulate small molecules or particles for drug delivery are most traditional, this talk shows the splendid potential of polymersomes to study viscoelasticity and shape transformations in two dimensions, with possible future applications for future biomechanics and soft robotics.

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발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 유자형

Functional thermo-responsive Poly(2-oxazoline)s

장우동

연세대학교 화학과

Poly(2-oxazoline)s (POxs) are well-known thermo-responsive polymers that exhibit reversible hydrophilic–hydrophobic phase transitions at the lower critical solution temperature (LCST). Using living cationic ring-opening polymerization, various functional groups can be introduced into POxs. Several clickable POxs with propargyl or azide end groups have been designed and subsequently reacted with various functional groups to prepare multifunctional POxs that respond to stimuli such as temperature, pH, chemicals, and light. In this symposium, I would like to briefly introduce recent approaches for clickable POx-based functional stimuli-responsive polymers and related applications.

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발표분야: Recent Trends in Polymer Synthesis: Supramolecular Polymerization

발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 유자형

Light-controlled self-assembly and polymerization of triphenylamine derivatives with supramolecular chirality

서명은

KAIST 나노과학기술대학원

Self-assembly of molecules via noncovalent interaction offers a fascinating route to construct organic nanomaterials by a “bottom-up” approach. The process requires to use of molecules with deliberately designed shape and functionality so they assemble following the information encoded in the molecular structure. Inducing a conformational change of the molecule by applying an external stimulus such as light can provide a new dimension on molecular self-assembly, enabling control of the self-assembly process with human intervention. In this talk, I will show the entire process of induction, control, and locking of supramolecular chirality can be manipulated by circularly polarized light (CPL), where the inherent chiral information encoded in the light is transferred into self-assembled aggregates. Taking a family of triphenylamine-containing molecules as an example that self-assembles in a solution and forms helical stacks upon light exposure, I will discuss control of the self-assembling behavior by controlling wavelength and rotational direction of the CPL.

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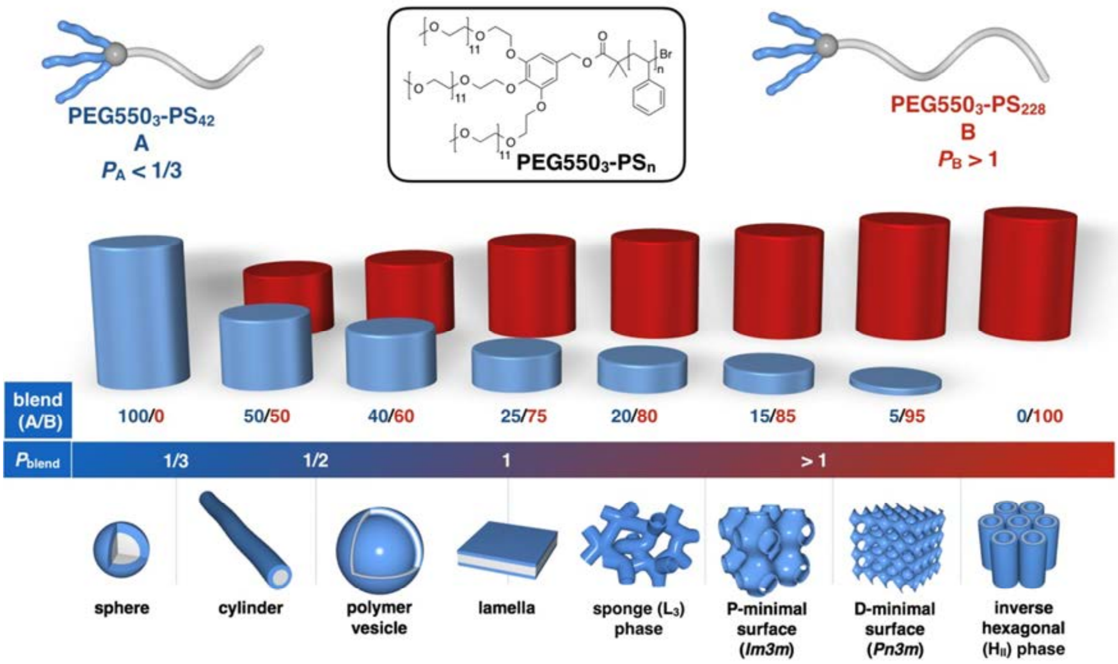
Mix-and-Match Assembly of Block Copolymer Blends in Solution

김경택

서울대학교 화학부

The chemical structure of a block copolymer (BCP) dictates the size, shape, and function of its self-assembled structure in solution. This direct correspondence demands precision synthesis of a specific BCP with optimized structural parameters to obtain the desired nanostructures with structural and functional complexity by solution self-assembly. Here we show that the binary blends of BCPs self-assemble into the desired nanostructure in solution by adjusting the composition of the blend. By modifying the structural parameters of a binary BCP blend through control of the composition, two BCPs sharing the repeating units in both polymer blocks co-assemble into the desired structures, which range from spherical micelles to inverse cubic and hexagonal mesophases. These BCP blends not only allow the direct creation of complex periodic mesoporous structures of the desired periodicity and pore size, but also provides nanostructures of unprecedented morphology by simple solution self-assembly without relying on the synthesis of correspondingly designed BCPs.


PEG550$_3$-PS$_{42}$
A
$P_A < 1/3$
PEG550$_3$-PS$_n$
PEG550$_3$-PS$_{228}$
B
$P_B > 1$
blend (A/B)
100/0
50/50
40/60
25/75
20/80
15/85
5/95
0/100
P_{blend}
1/3
1/2
1
> 1
sphere
cylinder
polymer vesicle
lamella
sponge (L$_3$) phase
P-minimal surface (*Im3m*)
D-minimal surface (*Pn3m*)
inverse hexagonal (H$_{II}$) phase

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Supramolecular protein oligomers with new structures and functions

정용원

KAIST 화학과

Supramolecular protein assemblies offer novel nanoscale architectures with molecular precision and unparalleled functional diversity. A key challenge, however, is to create precise nano-assemblies of functional proteins with both defined structures and a controlled number of protein building blocks. In this talk, I will introduce several new strategies to fabricate large protein assemblies, which can be valuable assets to study multivalent interactions in nature. In particular, modifications and applications of fluorescent proteins and avidin proteins with highly interesting binding properties will be discussed. In addition, several examples of how newly fabricated biomolecules with multivalent interactions that can be applied for designing new bioanalytical or biointerfacing methods will be discussed.

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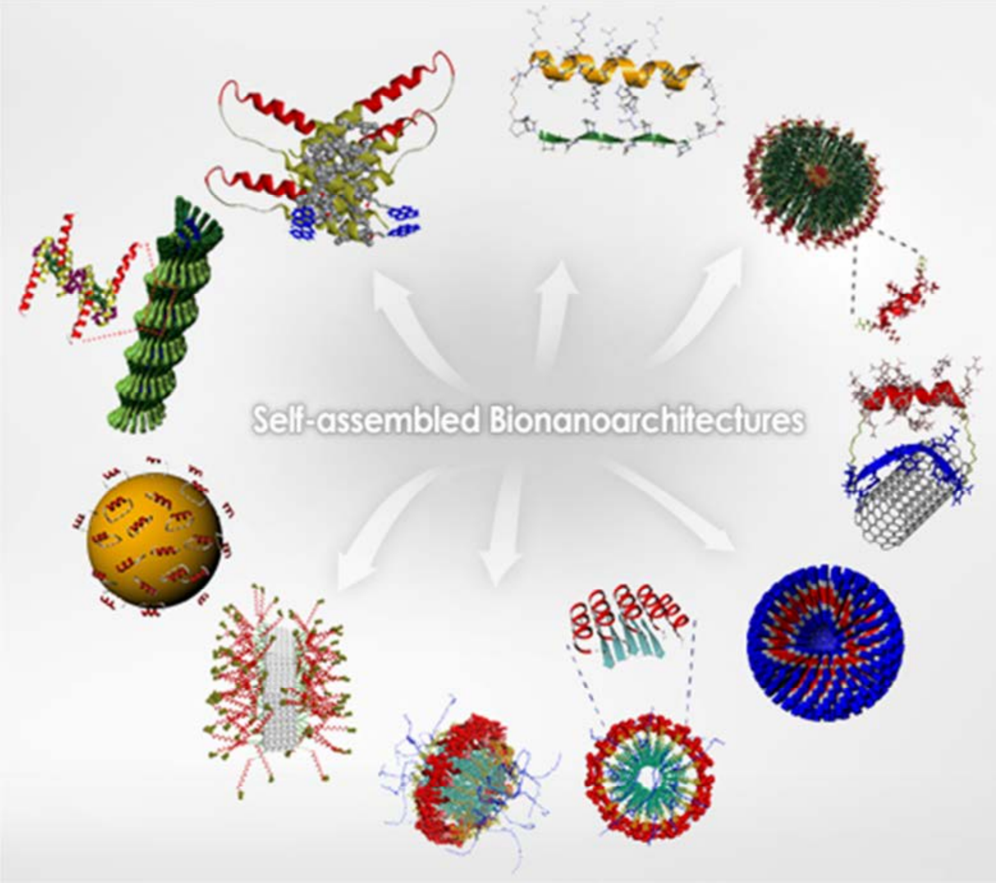
Unusual biological supramolecular assembly of peptides and peptide-DNA conjugates

임용범

연세대학교 신소재공학과

In recent years, interest in manmade or artificial bionanostructures, including peptide-based supramolecular assemblies have been intense and are expected to escalate further. Proteins are perhaps one of the most diverse and complex structures in nature. When designed appropriately, self-assembling peptide nanostructures (SPNs) can mimic the functions of natural proteins. This research group intends to develop SPNs that can mimic or even have enhanced functional properties over biological proteins. Moreover, we expect that SPNs can be designed to have properties that are unprecedented in nature. Since the major driving forces that underlies the formation of supramolecular assembly are noncovalent interactions and thermodynamic/kinetic principles, an elaborate design of supramolecular building block is an initial but the most critical step in controlled SPN formation. In this talk, our recent research efforts about the design of novel peptide-based building blocks, towards the understanding of unusual in-cell self-assembly behavior of peptides, and on the development of unique supramolecular assemblies of peptides and peptide-DNA conjugates, will be presented.


Self-assembled Bionanoarchitectures

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY3-6**
발표분야: Recent Trends in Polymer Synthesis: Supramolecular Polymerization
발표종류: 심포지엄, 발표일시: 금 16:05, 좌장: 박영석

3D nanoparticle assembly confined in supramolecular crystallization of block molecules

이은지

충남대학교 분석과학기술학과

양친매성 블록 분자에 동력학적 결합을 통해 결정성을 수반할 수 있는 블록을 도입하면 용액상 자기조립 과정을 통해 형태학적으로 다양한 나노구조체를 제조할 수 있고, 강한 콜로이드 안정성을 기대할 수 있다. 따라서 이러한 초분자 결정성을 제어 하는 것은 구조 및 물성의 다양성을 유도할 수 있다는 점에서 매우 흥미로운 나노기술이라 할 수 있다. 또한, 최근 독특한 광전기 특성을 지니는 무기 나노입자의 도입을 통해 소재적 관점에서 유기 나노구조체가 가지는 유연성, 공정 비용 절감, 가공성 등의 장점을 극대화 시키고자 정밀한 자기조립 제조 기술을 통해 하이브리드 나노소재를 만들고자 하는 다양한 노력들이 제시되고 있다. 본 강연에서는, 다양한 차원에서 하이브리드 나노구조체의 형태학적 특성에 기인하는 무기 나노입자와 블록 분자의 경쟁적인 자기조립 과정을 소개하고자 한다. 특히, 블록분자 조성 인자, 용매 선택성 등을 제어함으로써 블록 분자의 초분자 자기조립 결정화 과정을 통해 형성된 일차원, 삼차원 하이브리드 나노구조체 내부에서 무기 나노입자의 삼차원적 위치를 정밀하게 제어하는 방법을 소개하고자 한다. 나아가 하이브리드 나노구조와 물성의 상관관계를 설명하기 위한 삼차원 투과전자현미경 분석법을 소개하고 나노입자와 블록분자의 특성에 따라 전기광학적, 바이오메디컬 응용 가능한 사례를 소개하고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND1-1**
발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅰ
발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 백진욱

Photocatalyst/Biocatalyst Integrated Artificial Photosynthesis System for Highly Selective Solar Fuel/Chemical production

백진욱

한국화학연구원 인공광합성연구그룹

The natural photosynthetic process has fascinated chemists for long due to its high specificity in solar energy conversion to sugar. However, given the structural and functional complexity, it is a challenge to mimic this natural process. Nonetheless,efforts to develop efficient photosynthesis mimetic systems have been going on since 1970s. In recent years, these efforts have intensified due to increasing emphasis on the development of carbon-free or carbon-neutral systems/technologies for production of solar fuel/chemicals. Utilizing the natural photosynthesis as blueprint, a number of covalent, and non-covalent donor-acceptor conjugate dyes have been studied as systems for CO2 fixation. Although capable of efficient photoinduced intra- and intermolecular electron transfer (ET), they suffer from poor conversion efficiency and lack photostability. For enhanced efficiency and photostability, a variety of photocatalytic materials, such as inorganic frameworks and metal complexes have been developed and evaluated. However, their direct utilization remains limited due to one or more reasons, which include, low efficiency, poor selectivity, limited photostability and inability to work in visible light. This has led to emergence of the coupling of a suitable visible light active photocatalyst to an enzyme as an exciting avenue of research in this area. In this regard, we developed the photocatalyst/enzyme integrated solar chemical factory platform system that exemplified solar energy in synthesis of solar fuel & solar chemicals. The present work demonstrates successfully a new and potentially promising solar chemical factory platform system for the ultimate goal of utilization of solar energy in fuel & fine chemical synthesis.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **IND1-2**

발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅰ

발표종류: 심포지엄, 발표일시: 목 09:30, 좌장: 백진욱

Dye-Sensitized Hybrid Photocatalyst for CO2 Reduction

손호진

고려대학교 신소재화학과

Alarmed by global warming, and apprehended by unbridled green-house gas emission, we are facing a great challenge on climate change; thus, the reduction of CO2 gas and further to the conversion of CO2 have been the major research topics both in academics and industries.[1] Recently, the photochemical multiple-electron reduction of CO2 represents a reliable method of producing useful chemicals, converting CO2 to organic feedstocks such as carbon monoxide (CO), formic acid (HCOOH, 2 electron reduction), methanol (CH3OH, 6 electron reduction), and methane (CH4, 8 electron reduction).[2] We have developed efficient organic and inorganic hybrid phtocatalytic system involving three major components that will eventually converge to a unified hybrid system to become a “dye-sensitized semiconductor hybrid” photocatalyst.[3] Initial solar light sensitization occurs at the photosensitzer (PS) followed by electron transfer to the n-type semiconductor (n-SC), most commonly at TiO2 and finally to the site of organometallic molecular reduction catalyst (RC), facilitating the generation of electrons that can be funnelled to RC, where they will react with CO2. A cartoon that represents our hybrid photocatalyst system is shown in Figure. In the course of further optimizing the current dye-sensitized photocatalytic CO2 reduction, several strategies were employed with the introduction of diverse types of sensitizers showing light-harvesting ability in long-wavelength region and alternate reduction catalysts (Ru, Ni, Mn-based organometallic complexes).

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **IND1-3**

발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅰ

발표종류: 심포지엄, 발표일시: 목 10:00, 좌장: 백진욱

태양에너지의 화학적 연료 변환을 위한 염료감응형 광전합성소자

(Dye-Sensitized Photoelectrosynthesis Cell (DSPEC) for Solar Fuel Production)

위경량

대구대학교 화학응용화학과

In this presentation, we will introduce an artificial photosynthesis system for the solar fuel production from the water. Among the various artificial photosynthesis systems, we are focusing the dye-sensitized photoelectrochemical cell (DSPEC), which is molecular level light absorption and oxidation (or reduction) catalyst approaches. In the DSPEC, 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: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND1-4**
발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅰ
발표종류: 심포지엄, 발표일시: 목 10:30, 좌장: 백진욱

Artificial Photocatalytic Systems for Cofactor Regeneration and Carbon Dioxide Reduction

김진홍* 김수진 전유정[1] **TIKUM FLORENCE ANJONG**[2]

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학나노과학과 무기화학전공

For the practical use of a photo-bioreactor for artificial photosynthesis, efficient visible light-absorbing materials have to link reduction and oxidation catalysts for an efficient energy flow. As a step toward this goal of an NADH regeneration system and enzymatic production of solar fuels from CO2, we report the synthesis of a new polydiacetylene compound that is covalently connected with [Ru(phen-NH2)(bpy)2]2+ (bpy = 2,2'-bipyridine, phen = 1,10-phenonthroline-5-amine). The [(bpy)2Ru(phen)]-polydiacetylene absorbed a wide range of visible light because of the presence of two chromophores, the Ru complex and polydiacetylene. The polyacetylene backbone was converted from blue to red by conformational changes under the catalytic reaction conditions in a buffer solution. The electron transfer from the photoexcited [Ru(phen)(bpy)2]2+ to the polydiacetylene backbone was observed. In a visible light-driven photocatalytic NAD+ reduction by (cyclopentadienyl)Rh(bpy)(H2O)2+ with [(bpy)2Ru(phen)]-polydiacetylene, NADH was regenerated, and the reactivity using Ru(bpy)2(phen)-polydiacetylene was enhanced relative to control experiments using only [Ru(phen)(bpy)2]2+ or polydiacetylene. The consecutive carbon dioxide reduction coupled with formate dehydrogenase was carried out to utilize the in-situ photoregenerated NADH catalytically. The catalytic condition using [(bpy)2Ru(phen)]-polydiacetylene also showed much higher reactivity than the controls.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND2-1**
발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅱ
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 박현웅

Development of high efficiency Cu delafossite photocatalyst films for solar fuels

박현웅

경북대학교 에너지공학부

Photocatalysis uniquely mimics natural photosynthesis in terms of light absorption and conversion, as well as storage of the absorbed photon energy into chemical bond energy. Despite this similarity, the development of low cost photocatalysts capable of selectively producing liquid chemicals from CO2 and water with efficiency and durability comparable to those in typical photosynthesis remains a great challenge. Herein, we report the facile, environmentally benign synthesis of CuFeO2 and CuO binary films via electrodeposition, and demonstrate that these binary films produce only liquid formate from aqueous CO2 at ~1% energy efficiency, while driving O2 evolution from water on a wired Pt plate under continuous irradiation of simulated sunlight (AM 1.5G; 100 mW/cm2) over 24 h. An as-synthesized photocatalyst film with a three-dimensional, double-layer configuration further shows the continued production of formate for over 17 days. However, the crystalline structure and elemental state of the used photocatalysts undergo gradual chemical reduction. Such a deformation can be thermally healed by recycling the weekly used samples via oxidative annealing. Thus, a single photocatalyst sample produces formate continuously for 35 days.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND2-2**
발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅱ
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 박현웅

WO_3 based photoelectrochemical solar water splitting

박종혁

연세대학교 화공생명공학과

Tungsten Oxide is a good candidate as photoanode for photoelectrochemcial water splitting. According to the natural properties like band gap value, conductivity and surface chemical state, modifications should be conducted for WO_3 to improve the PEC performance. First, we designed 3D inverse opal structure for WO_3 and combined that with $BiVO_4$ for heterojunction structure, resulting dramatic improvement of PEC performance. Second, surface modification with overlayer was employed to improve the water oxidation property of WO_3. A WO_3 overlayer with dual vacancies prepared by using a solution-based reducing agent, Li-EDA (lithium dissolved in ethylenediamine), which improved the PEC performance of the mesoporous WO_3 photoanode dramatically. In comparison to the pristine samples, the interconnected WO_3 nanoparticles surrounded by a 2-2.5 nm-thick overlayer exhibited a photocurrent density approximately 2.4 times higher and a markedly cathodic shift of the onset potential, which is mainly attributed to the facilitative effect on interface charge transfer and the improved conductivity by enhanced charge carrier density. This simple and effective strategy may provide a new path to improve the PEC performance of other photoanodes.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **IND2-3**

발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅱ

발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 박현웅

CuInGaSe2 (CIGS) based photoelectrode for solar-fuel production

민병권

한국과학기술연구원(KIST) 청정에너지연구센터

Solar-fuel production inspired from nature has attracted substantial attention due to a need for developing sustainable future energy as well as chemical resources. In this study, we demonstrated a highly efficient solar energy to chemical conversion device using CO2 and water as feedstock. For the realization of this architecture we developed a thin film photovoltaic technology for the light absorbing component using a low cost, solution based Cu(InxGa1-x)(SySe1-y)2 (CIGS) fabrication method to provide high enough potential for the conversion reactions. This CIGS technology was also applied to photocathode fabrication for direct reduction of proton or CO2 in aqueous phase. The details of the synthetic method and characterization of each component and the solar-fuel production system will be discussed in the presentation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND2-4**
발표분야: Photocatalytic Water Oxidation and Carbon Dioxide Reduction Ⅱ
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 박현웅

Artificial Photosynthesis of CO2 Reduction into Liquid Fuels : Reduction Potential Tuning and Multi-electron Shuttling Process

강영수

서강대학교 화학과

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

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장소: 일산 KINTEX
발표코드: **IOMT-1**
발표분야: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] New Horizons in Inorganic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이광렬

Mesoporous zeolite catalysts

유 룡* 조창범 신혜선[1] 조장근[1] 좌진용[1]

기초과학연구원 나노물질및화학반응연구단 [1]KAIST 화학과

Zeolites are a family of microporous crystalline aluminosilicates, which are very important in catalysis. Over the past decades, microporosity was the main focus of the zeolite catalysis. Strong acid sites located on the micropore walls were the catalytic active sites for alkylation, isomerization, and cracking. The zeolite micropores were also supported with various kinds of transition metal catalysts to use in dehydrogenation, hydrogenation and oxidation. But since the discovery of MCM-41 mesoporous silica, mesoporosity emerged as a topic of interest in zeolite catalysis. Particularly in recent years, various types of microporous zeolite could be synthesized with a highly mesoporous morphology, using surfactants that were functionalized with zeolite structure-directing agents. Mesopores in these zeolites were disordered and interconnected to each other in a manner reminiscent of nanosponges. Despite the pore disorder, the zeolite nanosponges exhibited a narrow distribution of mesopore diameters, and also a large mesopore volume comparable to that of MCM-41. The mesopore walls in the zeolite nanosponges were ultrathin frameworks of microporous crystalline zeolite, and the wall surfaces possessed strong acid sites. The internal micropores inside the mesopore walls were accessible through apertures on the wall surfaces, resulting in rapid diffusion of reactants. This lecture begins with an overview of recent progress in the synthesis of mesoporous materials composed of microporous crystalline wall structures, using zeolite structure-directing surfactants. Then, we move to the characterization of acid catalytic properties of the mesoporous zeolites. Finally, we present new exciting results obtained by supporting transition metal catalysts in the zeolite mesopores.

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장소: 일산 KINTEX
발표코드: **IOMT-2**
발표분야: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] New Horizons in Inorganic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 14:05, 좌장: 이광렬

INTERFACING NANOMATIERALS FOR BIOMEDICAL INNOVATIONS

천진우

Institute for Basic Science (IBS) Center for Nanomedicine, Yonsei-IBS Institute Department of Chemistry, Yonsei University, Korea

One of the important trends of next-generation biomedical sciences is the development of new tools that can accurately image, identify, and execute desired missions in a selectively programed manner. Nanotechnology is among one of the essential platform tools for targeted imaging, therapy, and simultaneous monitoring of therapeutic efficacy. In this talk, I will discuss magnetic nanoparticles as a core platform material and tool for a variety of functionalities such as sensing, targeting and signaling of cells in a selective and efficient way. Their unique utilizations in highly accurate dual-modal MR imaging, therapeutic hyperthermia of cancer cells, controlled drug/gene delivery, and molecular level cell signaling and cell fate control will be discussed.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IOMT-3**
발표분야: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] New Horizons in Inorganic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 주상훈

Dynamic nanoscale surfactants

Bartosz Grzybowski

UNIST IBS첨단연성물질연구단/화학과

Surfactants are typically molecules whose key role is to lower the surface tension between liquid phases. At the same time, surfactants have not been considered as active elements that can set the liquids on motions or drastically alter their properties. In my talk, I will describe two new classes of surfactants based on appropriately functionalized nanoparticles or MOFs. These surfactants can be made responsive to various external fields (optical, magnetic, electric), can be used to manipulate, rotate, and assemble the droplets they enclose, and can stabilize droplets of very complex, non-spherical shapes. In one remarkable demonstration, our “nanosurfactants” are strong enough to actively pump the liquid they enclose out, into an immiscible outer liquid phase. All in all, nanoscale synthesis allows for the creation of completely new types of dynamic surfactant species, that are capable of change and also of performing useful work.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IOMT-4**
발표분야: [Inorganic Chemistry - Materials Chemistry Divisions Joint Symposium] New Horizons in Inorganic Nanomaterials
발표종류: 심포지엄, 발표일시: 목 15:15, 좌장: 주상훈

Dynamic Responsive Nanostructures Fabricated by Self-Assembly

박소정

이화여자대학교 화학나노과학과

Here, we present two-different approaches for the fabrication of shape-shifting DNA nanostructures. Firstly, dual-responsive DNA block copolymer was synthesized by coupling a thermo-responsive polymer, poly(N-isopropylacrylamide (PNIPAM) and an oligonucleotide. DNA-b-PNIPAM possesses thermo-responsive properties of PNIPAM as well as molecular recognition properties of DNA. DNA triblock copolymers of DNA-b-PNIPAM-b-PMA was also synthesized by introducing a hydrophobic block, poly(methyl acrylate) (PMA) to DNA/PNIPAM block copolymers, which form spherical micelles at room temperature. DNA-b-PNIPAM-b-PMA micelles undergo sphere-to-cylinder shape changes above LCST due to the conformational change of PNIPAM. The low temperature spherical morphology can also be accessed by introducing complimentary DNA strands. These results demonstrate the multi-dimensional shape changing capability of DNA-b-PNIPAM-b-PMA enabled by their dual-responsive property. Secondly, shape-shifting nanoparticle films were fabricated by combining the layer-by-layer thin film fabrication method and DNA-based self-assembly. We demonstrate that the nanoparticle thin films can undergo complex shape transformations under various external stimuli including DNA strands.

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장소: 일산 KINTEX
발표코드: **INOR1-1**
발표분야: Self-assembly of Inorganic Molecules and Nanoparticles
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 박소정

Chiral Arrangement of Achiral Inorganic Nanoparticles by Supramolecular Assembly of Helical Nanofiber Templates

정종화

경상대학교 화학과

Chiral materials comprised of organized nanoparticle superstructures have promising applications to photonics and sensing. Reliable customization of the chiroptical properties of these materials remains an important goal; hence, we report a customizable scheme making use of modular gelator components for controlling the helicity and formation of nanofibers over long length scales resulting in hydrogel templates. Controlled growth of gold nanoparticles at spatial-ly arranged locations along the nanofiber is achieved by UV reduction of Au(I) ions on the supramolecular templates. The resulting materials were found to have significant inter-particle interactions and well defined helicity to provide high quality, chiroptically active materials. With this novel approach, the tailored assembly of nanoparticle superstructures with predictable chiroptical properties can be realized in high yield, which we expect to allow rapid advancement of chiral nanomaterials research.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR1-2**

발표분야: Self-assembly of Inorganic Molecules and Nanoparticles

발표종류: 심포지엄, 발표일시: 금 09:30, 좌장: 박소정

Fabrication of Gold Nanoparticles into Hierarchical Structures with Amyloidogenic Protein of α-Synuclein

백승렬

서울대학교 화학생물공학부

Fabrication of nanoparticles (NPs) into multi-dimensional structures is crucial for maximizing the physical and chemical properties of individual NPs to be applied in the development of high-performance nano-devices. Here, gold-nanoparticles (NPs) have been assembled with an amyloidogenic protein of α-synuclein (αS), the major pathological component of Lewy bodies found in the degenerating neurons of Parkinson's disease. By taking advantage of the unit-assembly process of αS, AuNPs coated with αS were assembled into either anisotropic 1-D chain or tightly packed single-layered 2-D array on a chemically diverse set of substrates. The resulting peapod-type AuNP chains embedded within the amyloid protein nanofibrils were shown to be capable of exhibiting photoconductance with visible-light. The αS-mediated single-layered AuNP adsorption was also employed in surface-enhanced Raman scattering (SERS)-based biosensor development, non-volatile memory development, fuel-cell performance improvement, plasmonic solar-cell enhancement, and photodynamic cell-culture platform fabrication, where the outlying αS has played versatile roles. In addition, the tightly packed 2-D AuNP array was successfully unleashed from a substrate of polycarbonate in the form of free-floating monolayer film showing unlimited expandability, robustness for patterning, and flexibility leading to conformal contact. Not only these approaches, therefore, offer a facile and general way to fabricate NPs into hierarchical structures, but also the unique properties provided by the protein sheath make the resulting hybrid structures multi-functional photoelectric fusion materials suitable for applications in future nano-bio-technology.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR1-3**

발표분야: Self-assembly of Inorganic Molecules and Nanoparticles

발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 박소정

Sequentially Self-Limited Molecular Layer Deposition of Uniformly Aligned Polymer Films

이진석

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 presentation, I will present uniformly aligned polymer MLD films by repeating alternative vapor exposures of 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 polymer MLD films, which corresponded well with density functional theory (DFT) calculations. Furthermore, the polymer MLD films were fabricated using different carbon chain length and bond type of hydrocarbons to compare the molecular orientations of thin film, which investigated by grazing incidence wide angle X-ray scattering (GIWAXS).

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장소: 일산 KINTEX

발표코드: **INOR1-4**

발표분야: Self-assembly of Inorganic Molecules and Nanoparticles

발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 박소정

Self-Assembly of Reconfigurable 3-Dimensional Chiral Nanostructures with Optical Activity in Visible Range

염봉준

명지대학교 화학공학과

Natural materials behold innate handedness or chirality, for example, in the L or D forms of amino acids and twisted double helix of DNA molecules. However control of handedness in artificial materials is still challenging, especially for chiral nanomaterials. Chiral nanomaterials possess mirrored geometries that are lack of translation and rotation symmetry in 3-dimensional spaces in nanoscale. Therefore preparations of such chiral materials were only achieved via advanced lithography with high cost and complicated process via self-assembly of DNA molecules. Here we present a facile route to self-assemble 3D chiral nanostructures with controllable optical activity in the visible range without using any lithography or intrinsic chiral biomaterials. The chiral nanocomposite films with plasmonic nanoparticles can be reversibly deformed to have preferred absorptions of circularly polarized lights via modulation of in-plane axial strain. We believe that the artificial chiral nanomaterials have potential to be applied in advanced applications such as photoelectronic devices and metamaterials in optical devices.

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장소: 일산 KINTEX
발표코드: **INOR2-1**
발표분야: Recent Trends in Solid State Chemistry
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 유원철

Structure-Property Correlation of Metal Hydroxides and Their Composites

정덕영

성균관대학교 화학과

The charged layers of metal hydroxides provided the multifunctional interface characteristics required to assemble the functional particles, resulting in the binary hybrid structures of inorganic-inorganic, polymer-inorganic or bio-inorganic composites. The mixing of colloidal solutions of metal hydroxides and polymer led to the formation of bulk-type polymer-inorganic composites after the melting of the polymer phase, where the polymer was homogeneously coated over the hydroxide without the phase segregation. A biomimetic multifunctional nanocomposite was synthesized, in which polymer thin film was deposited on metal hydroxide. Kinetic controlled polymerization provided a synthetic pathway for the nanostructured polymer-inorganic composites without polymer agglomerates, allowing the crystallinity of the pristine metal hydroxide nanoparticles to be maintained. The catalytic activity of polymer containing and platinum nanoparticle-metal hydroxide composites was evaluated by observing the reduction of p-nitrophenol, in which the polymer layer acts as a protection layer against surface contamination of the nanocomposites. The nanostructure of polymer-hydroxide composites drove the incorporative organic-inorganic functional materials with blocked surface and improved electrochemical properties, providing a reliable synthetic pathway to prepare multifunctional nanohybrid materials. This new nanostructure improved the rate of reaction, turnover frequency and reaction durability of catalysts without significant loss in conversion efficiencies.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR2-2**
발표분야: Recent Trends in Solid State Chemistry
발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 유원철

3D Porous Inorganic Nanowire Aerogels and Their Applications

정성미

한국화학연구원 미래환경연구센터

Creating 3D porous inorganic nanowire aerogels using various materials and inexpensive means remains an outstanding challenge despite their importance for many applications. Here, we present a facile methodology to enable highly porous inorganic nanowire aerogel production on a large scale and at low cost. The aerogels are obtained from in situ hydrothermal synthesis of one dimensional (1D) nanowires that directly form a cross-linking network during the synthesis process. Such a method not only offers great simplicity but also allows the interconnecting nanowires to have much longer length. The longer length offers aerogels with remarkable porosity and surface area extremely low densities are mechanically robust, and can have superelasticity by tuning the synthesis conditions. The nanowires in the aerogels serve both as structural support and active sites which greatly augmented their applications in environmental, catalysis, sensing, absorption, energy storage, and beyond.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **INOR2-3**
발표분야: Recent Trends in Solid State Chemistry
발표종류: 심포지엄, 발표일시: 금 15:20, 좌장: 유원철

Exceptionally off-stoichiometric Bismuth Telluride compounds for thermoelectric applications

정인

서울대학교 화학생물공학부

Thermoelectric technology directly converts waste heat into electricity and is considered a promising means of sustainable energy generation. While most of the recent advances in the enhancement of the thermoelectric figure of merit (ZT) resulted from a decrease in lattice thermal conductivity by nanostructuring, there have been very few attempts to enhance electrical transport properties, namely, power factor. We employed nanochemistry to stabilize bulk Bi2Te3 that goes beyond phase equilibrium, i.e., phase-pure n-type K0.06Bi2Te3.18. Incorporated potassium and tellurium in Bi2Te3 far exceeds their solubility limit, leading to simultaneous increase in the electrical conductivity and the Seebeck coefficient along with decrease in the thermal conductivity. Consequently, a high power factor of ~43 W cm–1 K–2 and a high ZT > 1.1 at 323 K are achieved. Our current synthetic method can be used to produce a new family of materials with novel physical and chemical characteristics for various applications.

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발표코드: **INOR2-4**
발표분야: Recent Trends in Solid State Chemistry
발표종류: 심포지엄, 발표일시: 금 15:45, 좌장: 유원철

Solution-Processed Fabrication of Multi-Functional Thin-Films using Colloidal Nanocrystal Inks

백태종

중앙대학교 융합공학부

Colloidal nanocrystals are widely used in various applications such as electronic devices, phosphors, lasers, magnets, and catalysts. The synthesis of highly uniform nanomaterials with controlled size, shape, and compositions is paramount to precisely understand their size-, shape-dependent physical and chemical properties. In addition, to arrange them into highly ordered arrays allows for designing multi-functional thin-films with novel collective behaviors. Here, I will describe novel materials chemistry to synthesize highly uniform nanocrystals with precise control of the size, shape, and compositions and integrate them into functional thin-films using solution-based fabrication technique. I will introduce the self-assembly of colloidal nanocrystals with controlled orientation and spatial distribution, which may allow the design of novel functional and hierarchical materials with novel collective properties.,

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장소: 일산 KINTEX

발표코드: **PHYS1-1**

발표분야: Physical Chemistry of Materials

발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 팽기욱

Coherent Multidimensional Spectroscopy

조민행

고려대학교 화학과

Multi-dimensional optical or vibrational spectroscopy is a special class of time domain nonlinear optical spectroscopy that employs multiple ultra-fast laser pulses to obtain information about the couplings between quantum states in a variety of molecular or condensed matter systems. Since these couplings are often sensitive to the detailed structural configuration of the active molecules and the overall dynamical system evolution including interactions with the local environment, a great deal of information can potentially be obtained. It is especially well suited to follow the evolution of quantum coherences in light initiated reactions, including photosynthesis, or as an exceptionally useful probe of protein dynamics in solution. In fact, as demonstrated over the years, a vast number of different experimental configurations are possible depending on the chosen pulse sequences, geometric arrangement and polarization and signal detection method. Hopefully, this talk imparts a sound conceptual basis that might help any diligent researchers to understand the importance of this extensive and rapidly growing research field.

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장소: 일산 KINTEX
발표코드: **PHYS1-2**
발표분야: Physical Chemistry of Materials
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 팽기욱

A study on two-dimensional materials for energy harvesting with first-principles calculations

신영한

울산대학교 물리학과

As the electronic devices become smaller, all the components inside the devices need to be decreased.Random access memories are already in a nanoscale, and smart phones are in a race against the thickness. When the components are getting smaller and smaller, the materials for these components face problems such as leakage currents and stability. The well-known two-dimensional material, graphene, has been regarded as a promising material for electrodes due to its zero band gap. However, not only metallic but also semiconducting materials are required to compose electronic devices. Piezoelectricity can be obtained for dielectric materials, and electrolytes need insulating properties. To make graphene semiconducting, many methods were developed, and one of them is the functionalization. Researchers also found that other two-dimensional materials such as MoS_2 and SnS_2 are intrisically semiconducting. Focussing on the band gap tuning, piezoelectricity, ferroelectricity, and ion transport,[1,2,3] I will show physical and chemical properties of a series of two-dimensional materials that my research team has been studied in recent several years by using density functional theory calculations.

[1] A. Samad, M. Noor-A-Alam, and Y.-H. Shin, J. Mater. Chem. 4, 14316-14323 (2016).
[2] M. Noor-A-Alam and Y.-H. Shin, Phys. Chem. Chem. Phys. 18, 20443-20449 (2016).
[3] M. Noor-A-Alam, H.J. Kim, and Y.-H. Shin, J. Appl. Phys. 117, 224304 (2015).

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS1-3**
발표분야: Physical Chemistry of Materials
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 팽기욱

The photophysical mechanisms for the upconversion in lanthanide-doped upconverting nanoparticles (UCNPs)

이강택

GIST 물리화학부 화학과

Lanthanide-doped upconverting nanoparticles (UCNPs, NaYF4:Yb3+,Er3+) are well known for emitting visible photons upon absorption of two or more near-infrared (NIR) photons through energy transfer from the sensitizer (Yb3+) to the activator (Er3+). Of the visible emission bands (two green and one red band), it has been suggested that the red emission results from two competing upconversion pathways where the non-radiative relaxation occurs after the second energy transfer (pathway A) or between the first and the second energy transfer (pathway B). However, there has been no clear evidence and thorough analysis on the partitioning between the two pathways. In particular, the photophysical pathways of the red emission have been controversial. We examined the spectra, the power dependence of UCNP emission by either 980-nm or 488-nm excitation, to address which pathway is preferred. In addition, we performed stimulated emission depletion measurements, of which the result indicates consistently that the pathway B is the predominant path for the red emission.

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발표코드: **PHYS1-4**
발표분야: Physical Chemistry of Materials
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 은창선

Photophysical Properties of Organic Dye-Encapsulated Polymeric Nanoparicles

곽민석

부경대학교 화학과

Among organic fluorophores 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. About 30 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.

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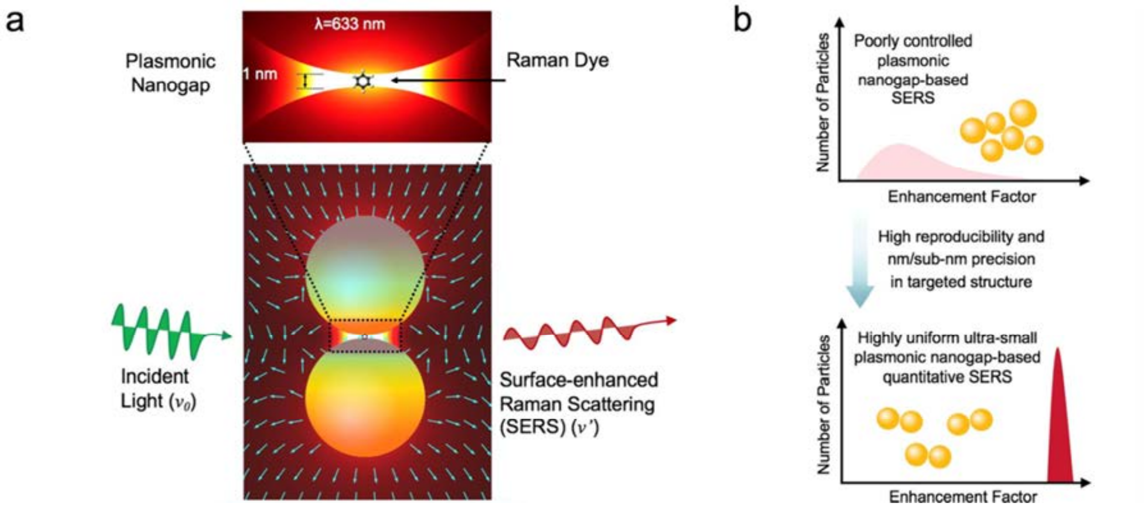
장소: 일산 KINTEX
발표코드: **PHYS1-5**
발표분야: Physical Chemistry of Materials
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 은창선

Physical Chemistry of Nanogap-Enhanced Raman Scattering (NERS)

서영덕

한국화학연구원/성균관대학교 나노라만융합연구센터/화학공학부

Raman scattering can provide a wealth of molecular chemical information, but it is basically a highly inefficient inelastic light scattering process between photon and molecule with a very small cross-section. Raman scattering signals are often poorly reproducible, meaning that very strong and controllable amplification mechanism, such as SERS(Surface-Enhanced Raman Scattering) or NERS(Nanogap-Enhanced Raman Scattering), is needed to obtain measurable and reliable Raman signals. Plasmonically coupled metallic nanostructures with ultra-small (～1 nm or smaller) nanogaps can generate very strong and controllable electromagnetic fields that can generate strong NERS signals from Raman dyes inside the nanogap. Therefore, plasmonic nanogap-enhanced Raman scattering (NERS) can be defined as Raman scattering signal enhancement from plasmonic nanogap with ～1 nm gap size. In this talk, I will overview recent breakthroughs, advances, application, and prospects of plasmonic nanogap-enhanced Raman scattering with metal nanogap particles revealed by single-molecule/single-particle-level Nano Raman spectroscopy showing that these plasmonic nanogap particles can generate ultra-strong, quantifiable Raman signals in a highly reproducible manner. References[1] H. Lee, S.M. Jin, H.M. Kim, and Y.D. Suh, Phys. Chem. Chem. Phys. (invited review article), 15, 5276 (2013).[2] D. Lim, K.-S. Jeon, H.M. Kim, J.-M. Nam, and Y.D. Suh, Nature Materials, 9, 60 (2010).[3] J.-H. Lee, J.-M. Nam*, K.-S. Jeon, D.-K. Lim, H. Kim, S. Kwon, H. Lee, Y.D. Suh, ACS Nano, 11, 9574 (2012).[4] H. Lee, G.-H. Kim, J.-H. Lee, N.H. Kim, J.-M. Nam, and Y.D. Suh, Nano Letters, 15, 4628 (2015).


a
λ=633 nm
Plasmonic Nanogap
1 nm
Raman Dye
Incident Light (v_0)
Surface-enhanced Raman Scattering (SERS) (v')
b
Poorly controlled plasmonic nanogap-based SERS
Number of Particles
Enhancement Factor
High reproducibility and nm/sub-nm precision in targeted structure
Highly uniform ultra-small plasmonic nanogap-based quantitative SERS
Number of Particles
Enhancement Factor

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장소: 일산 KINTEX
발표코드: **PHYS1-6**
발표분야: Physical Chemistry of Materials
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 은창선

Chemical and Orientational Imaging of Complex Polymeric Materials by Broadband CARS Microscopy

Young Jong Lee

National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

Broadband coherent anti-Stokes Raman scattering (BCARS) microscopy can provide label-free chemical images of biological and soft materials systems, faster than conventional spontaneous Raman microscopy. I demonstrate that appropriate polarization control of the high throughput imaging modality can capture both chemical composition and molecular orientation of complex polymeric materials, unraveling new information on the structure and rheology on the molecular scale. As an example, I discuss a study of a polyethylene (PE) blend that approximates the typical bimodal PE products, used for potable water and natural gas pipes. The study results in several new findings, which are unavailable by other conventional imaging methods. I will discuss them with respect to the mechanical failure mechanisms under mechanical stress and temperature. This new quantitative chemical and orientational imaging technique will help to understand the fundamental physics of complex polymeric materials and improve their physical properties.

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장소: 일산 KINTEX
발표코드: **PHYS2-2**
발표분야: Chemical Application of X-ray Free Electron Laser (XFEL)
발표종류: 분과기조강연, 발표일시: 금 09:30, 좌장: 이한주

Observing chemical dynamics on the atomic scale of time and space

Majed Chergui

Laboratoire de Spectroscopie Ultrarapide (LSU) and Lausanne Centre for Ultrafast Science (LACUS),
Ecole Polytechnique Fédérale de Lausanne CH-1015 Lausanne, Switzerland

The atomic scale resolution of space (the Ångström) was achieved a century ago with the discovery of X-ray and electron diffraction. It will take about 8 decades to reach the atomic scale of time (the Femtosecond) thanks to the pioneering works of Ahmed Zewail using optical domain spectroscopy. However, optical domain spectroscopies (ultraviolet, visible, infrared, Terahertz) do not deliver structure. Ultrashort pulses of electrons and X-rays have been used in recent years and I will focus on some of the landmarks leading to the development of the field of ultrafast structural dynamics with X-ray pulses. I will present results concerning molecular systems, proteins and transition metal oxides.

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발표코드: **PHYS2-1**
발표분야: Chemical Application of X-ray Free Electron Laser (XFEL)
발표종류: 분과기념강연, 발표일시: 금 09:00, 좌장: 이한주

Density-Corrected Density Functional Theory

심은지

연세대학교 화학과

Density functional theory (DFT) is used every research area that deals with materials yet there remain challenges where DFT suffers from the self-interaction error. We show that the energy error of any density functional calculation can be decomposed into errors contributed from the approximate functional and that from the self-consistent Kohn-Sham density. In vast majority of DFT calculations, the functional error dominates: however, we have found several abnormal cases where the density-driven error dominates. This analysis yields insights into the origins of many errors in DFT calculations, especially those often attributed to self-interaction or delocalization error. In many classes of problems, density-driven errors can be substantially reduced by using better densities. The density-corrected density functional theory (DC-DFT) is a non-variational DFT which uses more accurate density than the self-consistent approximate density. One of the simplest ways to implement the method is to use the Hartree-Fock density, i.e., HF-DFT, which has been already known to give remarkably accurate results in some cases including simple two electron atom energies, electron affinities of small molecules, dissociation curves, preferred geometries of ions and radicals in solution, spin-adiabatic energy of spin-crossover transition metal complexes, and more. In addition, the importance of being inconsistent in density functional calculations is discussed.

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발표코드: **PHYS2-3**
발표분야: Chemical Application of X-ray Free Electron Laser (XFEL)
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 이한주

4세대 방사광가속기 빔라인 및 레이저시스템 현황과 XFEL 연구를 위한 레이저 응용(Status of PAL-XFEL Beamlines and laser applications on XFEL sciences)

엄인태

포항가속기연구소 4세대 빔라인부

포항의 4 세대 방사광가속기 (이하 PAL-XFEL)는 미국의 LCLS 와 일본의 SACLA 에 이어 세계에서 3 번째로 운영이 시작될 X 선 자유 전자 레이저 (X-ray free electron laser, XFEL)이다. 2014 년 건물 완공 이후 주요 가속장치 및 빔라인 장치의 구축이 2015 년말 완료 되었으며, 2016 년 6 월 0.5 nm 자유전자레이저 발생을 시작으로 가속기 최적화와 빔라인 시운전을 거쳐 2017 년 하반기 이용자 지원을 시작을 앞두고 있다. 더불어 올해 1 월에는 연 X 선 자유전자레이저 발생에도 성공하여 현재 시운전 및 실험을 위한 준비가 진행 되고 있다.PAL-XFEL 에서 제공되는 광원은 펨토초 X 선 레이저로, 광자빔의 파장에 따라 0.6~0.06nm 영역의 경 X 선과 4.5~1.0nm 영역의 연 X 선으로 구분되며 초기에는 경 X 선 1 개 빔라인에 2 개의 end-station, 연 X 선 1 개 빔라인에 1 개의 end-station 이 각각 설치되어 운영된다. 실험적으로 XFEL 이 가져온 가장 큰 변화는 펨토초 수준의 짧은 펄스를 이용한 극초고속 시간분해 동역학 연구가 X 선 영역에서 가능하게 되었다는데 있다. X 선을 이용한 다양한 측정 - 회절, 산란, 이미징 등 모든 영역 -에서 XFEL 을 이용한 시간분해 동역학 연구는 ‘펌프’ 펄스에 의해 순간적으로 만들어진 비평형 상태의 계가 이완 또는 변화하는 과정을 XFEL 을 이용하여 ‘탐침’하는 펌프-프로브 방법을 주로 이용한다. 현재 가장 많이 쓰이고 있는 펌프 광원은 펨토초 광학레이저 펄스이다. PAL-XFEL 의 실험용 광학레이저 시설은 경 X 선과 연 X 선 실험홀에 각각 1 실이 구축되어 있으며 레이저 시스템은 총 3 기로 각 end-station 당 하나의 펨토초 레이저 시스템이 할당 되어 있다. 레이저 시스템의 주요 장치는 모두 클린룸 환경에서 운영되며 실험을 위한 펨토초 레이저 펄스는 각 end-station 의 시료 위치까지 전송되어 XFEL 을 이용한 동역학 연구에 이용된다. 또한 펨토초 레이저 펄스는 XFEL 광원의 시간 지터(jitter)를 측정하여 실험 결과를 보정함으로서 실험의 시간분해능을 높이는데 결정적인 역할을 한다.본 발표에서는 4 세대 자유전자레이저(FEL), 실험을 위한 PAL-XFEL 의 빔 라인 시운전 결과와 준비 현황에 대한 소개와 함께, XFEL 을 이용한 동역학 연구에서 사용되는 실험용 광학레이저 시스템과 그 응용에 대해 말하고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS2-4**
발표분야: Chemical Application of X-ray Free Electron Laser (XFEL)
발표종류: 심포지엄, 발표일시: 금 10:20, 좌장: 이한주

Element Specific Probing of Transient Species Using Time-Resolved X-ray Spectroscopy

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Ultrafast core-level spectroscopy is unique in its ability to probe transient states of matter with chemical specificity of single atom species by exciting core-level transitions from highly localized initial states. This allows atom-specific views of valence charge density depending on the probed atomic species. Recent progresses in ab initio calculations of core-level spectra provide new interpretations with details on the transient structure and valence charge density of a molecular system. Here we have employed ultrafast X-ray spectroscopic method to probe the valence charge density of first-row transition metal complexes in solution via metal 2p- and nitrogen 1s-spectroscopies. The former directly probes the spin-state and valence charge density of the metal and its immediate chemical environment on ultrafast time-scales by dipole 2p → 3d transitions. On the other hand, the latter provides a “ligand view” of the valence charge density dynamics. These measurements are compared with ab-initio density functional theory (DFT) calculations. These approaches give the way to obtain comprehensive pictures of valence charge densities of transient species. The possible applications of ultrafast core-level spectroscopy at X-ray free electron lasers will be discussed.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS2-5**
발표분야: Chemical Application of X-ray Free Electron Laser (XFEL)
발표종류: 심포지엄, 발표일시: 금 10:40, 좌장: 이한주

Time-resolved photoelectron spectroscopy on charge transfer dynamics in organic solar cells

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Organic solar cells (OSCS) has been extensively investigated for the last decade owing to their low-fabrication cost, high potential of large-scale production and application of flexible devices. There has been a quite huge technical success of improving the efficiency and stability of OSCs. However, the exact process of light to current conversion has not been well established so far. The light to electricity conversion of OSCs initiated by light absorption of photo-sensitive donor polymer followed by electron-hole pair (exciton) generation and charge transfer from donor to acceptor polymer. The time-resolved photoelectron spectroscopy technique can directly evidence the dynamics of photo-induced charge-transfer process in OSCs. Here the experimental results performed at Advanced Light Source (ALS) will be presented as an example of the direct observation of the electron transfer from CuPc (donor molecule) to C60 (acceptor molecule) using time-resolved X-ray photoelectron spectroscopy. The pulsed light source is essential for the time-resolved photoelectron spectroscopy and the table-top laser driven High Harmonic Generation (HHG) enable the access to VUV and soft X-ray photo energies also in the laboratory. This opens a lot of new possibilities in many scientific research fields of physics and chemistry in lab-based research facilities. In the end, the working principles of HHG-based light source will be presented together with the recent experimental study on the improving the HHG efficiency using the mixtures of two rare gases (Ar and Ne).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS3-1**
발표분야: Recent Physical Chemistry Studies on Energy and Catalysis
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 송봉근

반도체성 유기 고분자의 초기 산화 거동에 대한 표면 물리 화학적 연구

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반도체성 유기 고분자는 유기 태양 전지 등의 에너지 및 전자소자 등 다양한 분야에서 응용될 수 있어 그 성질에 대한 연구가 물리화학 분야에서 많이 진행되고 있다. 특히, 반도체성 유기 고분자의 산화는 유기태양전지의 효율 감소와 밀접한 연관이 있어, 그 산화거동이 많은 관심의 대상이 되어 왔다. 본 연구에서는 다양한 담체 표면위에 증착된 반도체성 유기고분자 중 하나인 P3HT (Poly(3-hexylthiophene-2,5-diyl)) 의 가시광선 조사 하에서의 산화 거동에 대해서 광전자 분광법을 이용하여 분석하였다. P3HT 의 thiophene ring 의 S 가 부분적으로 산화가 되면서 P3HT 의 conformational distortion 이 일어나게 되며, 이는 물, 산소 분자들이 P3HT 층 사이로 침투하는 현상을 유발하여 궁극적으로 P3HT 의 흡광도를 감소시키는 역할을 하는 것으로 나타났다. P3HT 박막의 산화는 그 밑의 담체 구조에도 영향을 많이 받는데, P3HT 에서 가시광선의 흡수를 통해 형성된 전자-정공 쌍이 재결합을 유발하는 담체들은 전자-정공이 산소나 물과 반응하여 O2-, OH 라디칼등의 산화제의 형성을 방해하여 P3HT 의 산화를 억제하는 것으로 나타났다. 가시광선의 파장을 바꿔가며 P3HT 의 산화를 연구한 결과에서는 Blue, Green, RED Light Emitting Diode 를 이용한 실험에서 P3HT 박막의 표면 부근에서는 파장에 따른 각기 따른 산화거동을 보였으나, P3HT 내부의 산화는 파장에 영향을 크게 받지 않는 것으로 나타났다. 이러한 반도체성 유기 고분자의 산화거동과 광학적 성질의 변화에 대한 표면물리화학적인 연구 결과들은 유기 고분자의 안정성을 높이는 방법을 고안하는 데 기초 자료로 활용될 것으로 기대된다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS3-2**
발표분야: Recent Physical Chemistry Studies on Energy and Catalysis
발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 송봉근

Nanoparticle Catalysis

<u>안광진</u>

UNIST 에너지 및 화학공학부

Nanoparticles have been widely utilized as an excellent catalyst for many catalytic reactions. Specific interfaces derived from metallic nanoparticles and oxide supports greatly influence catalytic performance. Newly created interfaces between metal and oxide in nanocatalysts were proven by enhancing activity and selectivity toward desired products in catalytic oxidation reactions. The utilization of elaborately designed nanoparticle catalysts and their specific interactions opens new possibilities for understanding interesting catalytic phenomena and for developing next-generation catalysts and efficient catalytic processes exhibiting 100 % selectivity, maximal activity, and long-term stability.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS3-3**
발표분야: Recent Physical Chemistry Studies on Energy and Catalysis
발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 송봉근

Electronic structures of photo-catalytic activities of TiO2 nanoparticles

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We investigate 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 track the optical and electronic band gap of a set of (TiO2)n nanoparticles ranging from small non-bulk-like clusters with n=4, 8 and 16, to larger nanoparticles with n=35 and 84 derived from cuts from the anatase bulk crystal structure. As the difference between these two energy gaps (the exciton shift) tends to zero in the bulk we use the magnitude of this shift as an indicator of how bulk-like the electronic structure of our nanoparticles are and how it is affected by size and structure. Extrapolating our results to larger sizes we thus provide a rough estimate of the nanoparticle size at which the electronic structure will begin to be effectively bulk-like. Our results generally confirm that the electronic structure of the nanoparticles has a significantly more pronounced structure dependency than size dependency. We also show that the exciton state is thermodynamically favored over free charged species both in vacuum and in water. We also investigate the effect of oxygen vacancies in TiO2 nanoparticles, (TiO2)35, on the photo-catalytic activities. We tested all the possible single oxygen vacancies and compared the energy levels, and found the enhanced photo-catalytic activity by single oxygen vacancy is due to the apperance of intermediate states.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS3-4**

발표분야: Recent Physical Chemistry Studies on Energy and Catalysis

발표종류: 심포지엄, 발표일시: 금 15:40, 좌장: 김도환

Theoretical Investigations on Electrocatalytic Activities of Carbon-based Nanostructures for Energy Devices: HER/OER/ORR/IRR

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The function of most energy devices such as lithium ion battery (LIB), metal-air battery, fuel cell and DSSC is based on the electrochemical redox reactions of electrode materials, which is accompanied by phase transition of electrode materials or catalytic reactions on the surface of electrode materials. Compared to the importance of phase transition on LIB between lithiated and delithiated phases, catalytic redox reactions play a very important role on metal-air battery and fuel cell devices because catalytic oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are involved in those devices. In addition, hydrogen evolution reaction (HER) and I_3^-/I^- redox coupled reaction are key issues on hydrogen-based fuel cell and DSSC devices.Here, we would like to introduce the theoretical overpotential calculated by applying standard density functional theory in combination with the computational standard hydrogen electrode (SHE) model to HER/OER/ORR and IRR of energy storage and harvesting devices.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS3-5**
발표분야: Recent Physical Chemistry Studies on Energy and Catalysis
발표종류: 심포지엄, 발표일시: 금 16:00, 좌장: 김도환

Photoelectrochemical hydrogen evolution from water splitting using a CIGS photocathode

황윤정

한국과학기술연구원(KIST) 청정에너지 연구센터

에너지 저장체로 수소를 이용하여 연료전지에서 전력을 생산시키는 기술은 청정 기술로 많은 관심을 받고 있다. 그러나, 현재의 수소제조법은 제조 단계에서 이산화탄소를 발생시키기 때문에, 연료전지가 청정에너지로 널리 보급되기 위해서는 청정한 수소의 제조 기술이 필수적으로 개발되어야 한다. 이에, 태양광에너지를 이용하여 연료전지의 역반응인 물을 분해하여 수소를 제조하고자 하는 기술이 많이 개발되어왔다. 빛을 흡수하는 반도체 광촉매 전극의 개발은 태양광 물분해 효율 향상을 위해 매우 중요한 핵심 기술이며, 많은 경우 반도체 소재의 안정성 등의 이유로 금속 산화물이 많이 사용되어왔다. 특히, 물산화 반응의 과전압이 높기 때문에, n-type 의 금속 산화물 기반의 광촉매 개발이 활발하게 진행된 반면, 환원전극의 개발은 상대적으로 최근에서 많은 관심을 받고 있다. 본 발표에서는 태양광 흡수율이 뛰어나 태양전지 소재로도 널리 쓰이는 CIGS 를 수소제조 광환원 전극으로 개발한 연구 내용에 대해서 논의하고자 한다. 용액공정의 CIGS 는 결정성이 떨어진다는 단점이 있는데, 표면층의 도입으로 charge recombination 을 줄일 수 있고, 특히 투명전극 위에서 증착된 CIGS 박막은 물질 특성 이해에 좀 더 다양성을 제공할 수 있다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1-6**

발표분야: Recent Advances in Analytical Chemistry I: Advanced Materials and Instrument in Analytical Chemistry

발표종류: 분과기념강연, 발표일시: 목 15:20, 좌장: 차상원

Heavy Water Labeling : Extracting a Big Change from Small Variations

김태영

GIST 지구환경공학부

Mass spectrometry (MS) has revolutionized biochemical analysis in terms of sensitivity, specificity, and speed. A fundamental drawback of MS as an analytical technique is the poor ability of quantification. To overcome this limitation, stable isotope labeling has been extensively employed for both relative and absolute quantification based on MS. In most quantitative MS experiments, complete labeling of target analytes with a specific type of heavy isotope (e.g., ^{2}H, ^{13}C, or ^{15}N) is designed for simple distinction of isotope-labeled compounds from non-labeled counterparts in a mass spectrum. However, the use of isotope labeling is a cumbersome practice mainly due to high cost and long time to achieve complete labeling. An alternative method to introduce an isotope to biomolecules is indirect deuterium labeling via heavy water ($^{2}H_2O$) administration, which results in strikingly different patterns of mass spectra because of partial isotope enrichment. In this presentation, properties and characteristics of $^{2}H_2O$ labeling are discussed along with its limitations and challenges for applications in MS-based quantification studies.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1-1**
발표분야: Recent Advances in Analytical Chemistry I: Advanced Materials and Instrument in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 김주훈

Flow FFF with Mass Spectrometry for Proteomic and Lipidomic Analysis

문명희

연세대학교 화학과

Flow field-flow fractionation (FlFFF) is a separation method capable of size-sorting particles and biological macromolecules like proteins, DNA, cells, and etc. in an empty channel space without packing materials. During separation of macromolecules by FlFFF, eluting fractions of narrow size range can be collected and utilized for further biological analysis. In this presentation, recent efforts to incorporate mass spectrometry (MS) with FlFFF either by off-line or on-line will be described with applications to proteomic and lipidomic analysis. For the case of off-line combination of FlFFF and MS, subcellular and extracellular species were separated by sizes first and then the collected organelle fractions of different sizes can be further investigated for the proteomic and lipidomic analysis using nanoflow LC-ESI-MS/MS. A miniaturiaed FlFFF can be utilized for the direct hyphenation to MS via electrospray ionization (ESI) or inductively couple plasma (ICP). The former enabled one to have top-down analysis of lipids from lipoproteins without extracting lipids and the latter led us to analyze metals from metalloproteins in blood plasmsa proteome. This presentation introduces recent works on the proteomic/lipidomic analysis of urinary exosomes from prostate cancer patients and on the direct metal analysis of metalloproteins from plasmsa samples with lung cancer.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1-2**
발표분야: Recent Advances in Analytical Chemistry I: Advanced Materials and Instrument in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 13:50, 좌장: 김주훈

Investigation on variation of Raman spectral feature by change of particle size

정희일

한양대학교 화학과

The variation of Raman spectral feature with change of particle size has been systematically investigated. Both lactose powders and pellets composed of five different particle sizes were prepared for the examination. Uniquely in this study, three separate spectral acquisition schemes with different sizes in laser illumination and detection window were employed. In both samples, the distribution of Raman photons became broader with the increase of particle size, since mean free path of laser photons, average photon travel distance between consecutive scattering locations, became longer under this situation. In a meanwhile, the photon distribution was narrower in the pellets since individual particles were more densely packed in a given volume. In overall, physical characteristics of a sample determining the internal Raman photon distribution was surely the main factor influencing on Raman intensity. More notably, experimental configuration used for spectral acquisition was another crucial factor affecting the peak intensity, as exclusively investigated in this study. Monte Carlo simulation was effective to probe the photon distribution inside the samples and help to support the experimental observations

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1-3**
발표분야: Recent Advances in Analytical Chemistry I: Advanced Materials and Instrument in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 김주훈

Synchrotron Infrared spectroscopy and its applications

채복남

포항가속기연구소 산업기술융합센터

Infrared spectroscopy uses the fact that different functional groups absorb characteristic Infrared radiation, which is very useful tool to identify and study the molecular structure, chemical/physical properties and reaction pathway of materials. In addition, it is possible to collect all wavelengths simultaneously in Fourier-Transform Infrared (FTIR) spectroscopy and examine the different types of samples using various sampling accessories, this technology is widely used in the fields of physics, chemistry, biology, environmental analysis and etc.Today, most synchrotron facilities offer a port dedicated to infrared (IR) spectroscopy and infrared-microspectroscopy. The main advantage of synchrotron-based infrared spectroscopy is the brightness of synchrotron radiation source. The synchrotron radiation source provides brightness 2-3 orders of magnitude higher than a thermal (Black body radiation) infrared source [1,2]. Thus, synchrotron based infrared spectroscopy has allowed high spatial resolution (infrared micro-spectroscopy) and high spectral resolution, especially for low throughput technologies and far-infrared spectroscopy. Infrared beamlines are now facing an increasing demand of beamtime from various disciplines: Biology, biomedical applications, plant biology, Earth Science, Environmental science, Chemistry, Cultural Heritage, Archaeology and soft matter [1,2].Synchrotron-based infrared spectroscopy and its applications will be presented. In addition, the current status of infrared beamline of PAL will be discussed.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX

발표코드: **ANAL1-4**

발표분야: Recent Advances in Analytical Chemistry I: Advanced Materials and Instrument in Analytical Chemistry

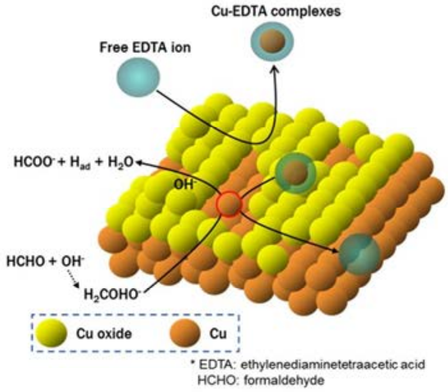
발표종류: 심포지엄, 발표일시: 목 14:40, 좌장: 차상원

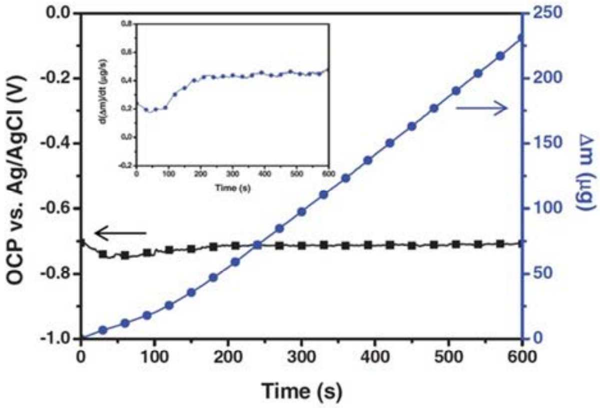
Real-Time Observation of Cu Electroless Deposition Process Using Electrochemical Quartz Crystal Microbalance

임태호

숭실대학교 화학공학과

반도체 공정은 구리 다마신 공정의 도입으로 기존의 배선 재료인 알루미늄을 구리로 전환하면서 혁신적인 발전을 이루었으며, 현재까지 집적도 증가와 적층 기술로 소자의 성능 향상을 도모하였다. 구리 배선 공정은 주로 구리 전해 도금으로 수행되며 이를 위해서는 도전 역할을 하는 균일한 구리 씨앗층의 형성이 필수적이다. 하지만 근래에 들어서 소자의 집적도 증가가 균일한 확산 방지층/구리 씨앗층 형성에 많은 문제점들을 야기하여 차세대 반도체 소자 제작에 어려움을 겪고 있다. 이러한 문제점들을 해결하기 위하여 원자층 증착법, 무전해 도금 등 기존 구리 전해 도금을 대체 또는 보완할 수 있는 다양한 방법이 고안되고 있다. 특히 구리 무전해 도금은 확산 방지층 위 구리 씨앗층을 균일하게 형성할 수 있을 뿐 아니라, 원자층 증착 방법을 이용한 루테늄 합금 또는 코발트 합금 계열의 차세대 확산 방지층 위에서도 구리 박막 형성이 가능하여 차세대 구리 배선 방법으로 주목 받고 있다. 하지만 구리 전해 도금과 달리, 도금 메커니즘이 복잡하고 단순 전기화학 분석 방법의 도입이 어려워 구리 무전해 도금의 메커니즘을 이해하는 데 많은 어려움이 있다. 본 발표에서는 개회로전압 측정과 수정진동자저울을 통해 전극의 무게 변화를 측정함으로써 구리 무전해 도금을 실시간으로 관찰할 수 있는 방법을 고안하였으며, 이를 통해 구리 무전해 도금의 메커니즘과 구리 무전해 도금에 사용하는 유기 첨가제의 흡착 거동 및 그 역할을 연구하였다. 우선, 구리 무전해 도금 용액을 구성하고 있는 착화제와 환원제가 구리 전극에 어떠한 영향을 미치는지 개별적으로 파악하였고, 구리 무전해 도금에서 널리 사용되고 있는 유기 첨가제인 polyethylene glycol (PEG), 2,2’-dipyridyl 그리고 3-N,N-dimethylaminodithiocarbamoyl-1-propanesulfonic acid (DPS)의 영향도 살펴보았다. 또한 유기 첨가제의 영향 연구를 바탕으로 60 nm 미만의 트렌치에서 구리 초등각 전착을 성공시켜, 차세대 구리 배선 방법으로의 구리 무전해 도금 적용 가능성을 확인하였다.


Cu-EDTA complexes
Free EDTA ion
HCOO⁻ + H_ad + H₂O
OH⁻
HCHO + OH⁻
H₂COHO⁻
Cu oxide
Cu
* EDTA: ethylenediaminetetraacetic acid
HCHO: formaldehyde


OCP vs. Ag/AgCl (V)
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
Δm (μg)
250
200
150
100
50
0
Time (s)
0
100
200
300
400
500
600
d(Δm)/dt (μg/s)
0.8
0.6
0.4
0.2
0.0
-0.2

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발표코드: **ANAL1-5**
발표분야: Recent Advances in Analytical Chemistry I: Advanced Materials and Instrument in Analytical Chemistry
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 차상원

Application of Electroanalytical Methods in Artificial Photosynthesis

안현서

연세대학교 화학과

Conversion of solar energy into transportable liquid fuels has been an important research theme in physical sciences for the last decade. Many artificial photosynthetic devices have been built with numerous iterations and enhancements, yet all fall short of the biological machinery. In the current presentation, two major problems in artificial photosynthesis will be discussed: 1) limited lifetime of the photo-absorber due to oxidative degradation and 2) deficient understanding of the complex oxygen evolution reaction (OER). In the first part of the presentation, a proof-of-concept photo-anodic device for OER will be demonstrated. Prolonged use of corrosion sensitive n-type silicon was made possible in water by application of an electrodeposited thin passivating layer of TiO2. A rare metal/insulation/semiconductor junction was employed for solution electrochemistry boasting an OER current density of 19 mA/cm2 that is indefinitely stable. In the second part of the talk, an investigation of the catalytic OER surface processes will be presented. By use of a redox titration experiment, the redox processes occurring at the surface of metal oxides during OER were investigated. The unique surface selectivity of the analytical technique employed here allowed for the selective data analyses of the processes occurring exclusively at the solid-solution interface independent from the participation of the signals from the bulk of the catalyst material. The results pertaining to the OER kinetic parameters and the key intermediates will be presented.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표분야: Recent Advances in Analytical Chemistry Ⅱ: Microfluidics for Novel Diagnostics
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 김상경

Applications of Digital Microfluidic Platform in Clinical Diagnostics

최기환

한국표준과학연구원(KRISS) 유기분석표준센터

Digital microfluidics (DMF) is a fluid handling technique in which discrete droplets are manipulated on the surface of an array of electrodes. The open nature of DMF systems enables the use of heterogeneous samples, such as dried blood spots and hydrogels. In this talk, I will present two recent projects using solid samples on a DMF device. First, I will describe the work implementing magnetic particle-based immunoassays in DMF. To increase the assay throughput, a new platform capable of performing complete immunoassays with minimal manual intervention was developed. This instrument comprises three core components: a Pogo pin interface for digital microfluidic control, an integrated photomultiplier tube for chemiluminescent detection, and an adjustable magnet for particle separation. Relative to macroscale methods, this DMF approach reduced reagent volumes and analysis time. Second, I will present an analytical technique to quantify the multiplexed steroid from tiny amount of tissue samples. Digital microfluidic actuation of methanol allowed to extract the analytes from milligram-sized tissue samples. The extractant was further processed in a DMF device with porous polymer monoliths prepared by photopolymerization of a C12 casting solution. The solution was injected and analyzed by HPLC-MS/MS for quantification of four hormones: estradiol, testosterone, androstenedione progesterone. This represents the first method capable of quantification of these analytes in core needle biopsy (CNB) samples, and suggests a future in which regular CNB testing is applied to a personalized medicine approach to diagnosis and treatment of hormone-sensitive cancer.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2-2**
발표분야: Recent Advances in Analytical Chemistry Ⅱ: Microfluidics for Novel Diagnostics
발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 김상경

Efforts to combine the digital microfluidics with advanced mass spectrometry

오한빈

서강대학교 화학과

In recent years, digital microfluidics (DMF) technology, which is based on electrowetting-on-dielectrics (EWOD) principle, has emerged as a powerful platform for the chemical and biological analysis. In DMF, a water droplet can be transferred into an adjacent electrode in a digitized (discontinuous) fashion through controlling electric potentials onto the electrodes. Through these controlled droplet movements, a droplet can be dispensed, split, merged, and transferred. These droplet manipulations enable one to do a variety of sample handling without human intervention, i.e., automation. In our laboratory, we have attempted to introduce the DMF technology into the mass spectrometry analysis. For example, DESI (desorption electrospray ionization) was utilized to analyze peptides, which were prepared by tryptic digestion of proteins of interest, on the DMF chip. In addition, sample preparation for phophopeptide analysis using MALDI-TOF MS was demonstrated to be implemented on the DMF chip platform. In the conference, recent results done in our laboratory will be introduced in detail.

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장소: 일산 KINTEX
발표코드: **ANAL2-3**
발표분야: Recent Advances in Analytical Chemistry Ⅱ: Microfluidics for Novel Diagnostics
발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 김상경

Wash-free magnetic immunoassay of hazardous materials using a fully automated SERS-based microdroplet platform

주재범

한양대학교 생명나노공학과

We report the rapid and sensitive immunoassay of hazardous materials using a surface-enhanced Raman scattering (SERS)-based microdroplet sensor. This sensor enables a convenient immunoassay of a specific marker without any washing process. Herein, magnetic immunocomplexes can be easily isolated by the droplet splitting into two smaller parts. One is the droplet including magnetic immunocomplexes and the other is the supernatant droplet including unbound SERS nano tags. In this system, droplet generation, transport, immunoreactions, isolation of immunocomplexes, droplet fission are sequentially performed to achieve a wash-free immunoassay in an automatic manner. SERS signals for unbound SERS nano tags in separated droplets were measured and analyzed for the quantitative analysis of a target marker. SERS signals for approximately 200 droplets/min (3.0 Hz) were measured and averaged for the quantitative evaluation of a target marker. In this system, a tiny volume of sample is needed since all the process can be automatically carried out in a specially designed microdroplet channel. We anticipate that this fully integrated SERS-based microdroplet device opens new insights in the development of a facile assay platform for various hazardous materials.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2-4**
발표분야: Recent Advances in Analytical Chemistry Ⅱ: Microfluidics for Novel Diagnostics
발표종류: 심포지엄, 발표일시: 금 15:55, 좌장: 김상경

Rapid Detection of Single Bacteria in Unprocessed Blood using Integrated Comprehensive Droplet Digital Detection

강동구

인천대학교 화학과

Antimicrobial resistance is a growing health problem in the United States and worldwide. According to the Centers for Disease Control and Prevention (CDC), more than two million people are infected annually with antibiotic-resistant infections, with >23,000 deaths. Aggressive bacterial infections associated with antimicrobial resistance are often managed within intensive care units (ICUs) with high associated costs, which impose significant healthcare, economic and social burdens.

Rapid diagnostics are particularly needed for pathogens such as E. coli, which are common, virulent, and have acquired ESBLs. Furthermore, diagnostic tests that can confirm the presence of ESBLs regardless of the species would be exceedingly valuable in directing early therapy and enabling better antimicrobial stewardship for those not infected with antibiotic resistant pathogens. Unfortunately, existing bacterial detection methods are limited in their inability to rapidly detect and identify pathogens that typically occur at low concentrations in blood (1 to 100 colony-forming unit (CFU)/mL) as is commonly found in adult BSIs. Conventional bacterial blood cultures coupled with susceptibility testing (automated methods or disk diffusion) require days to obtain a result. This lag in time to detect a patient with a culture positive BSI, identification of the isolate and establishing the antimicrobial susceptibility of the isolate contribute to the high mortality.

Here, we will discuss about our strategy for monitoring bacteria at single-cell sensitivity within a few hours by miniaturized droplet-based microfluidic system.

Key Words : Antimicrobial resistance, Lab on a chip, Microdroplet, Microfluidics, Digital quantification

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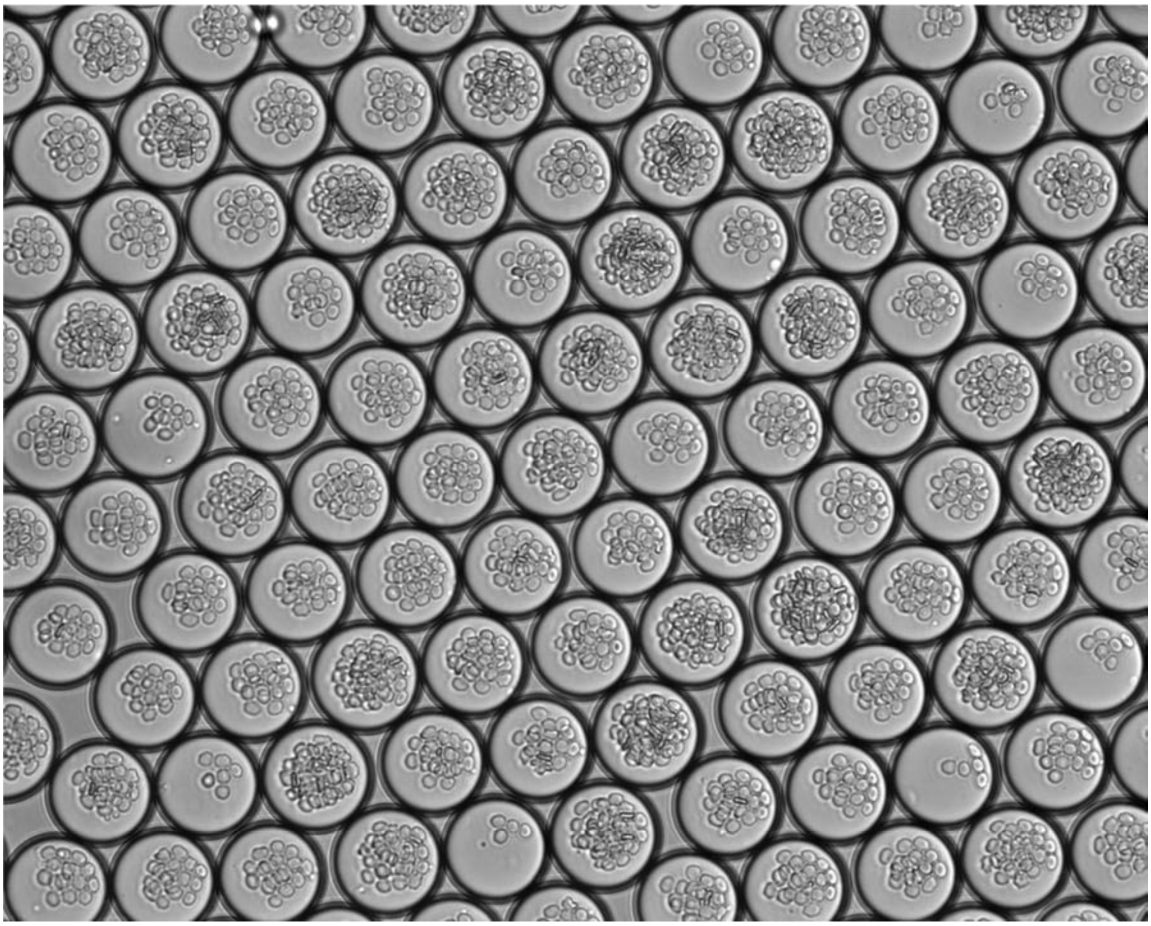
Encapsulated blood microcapsules



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장소: 일산 KINTEX
발표코드: **BIO1-1**
발표분야: Current Topics on Chemical Biology
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 기정민

Chemistry of proteins labeling for deciphering their functions in live systems

Itaru HAMACHI

Department of Synthetic Chemistry and Biological Chemistry Graduate School of Engineering Kyoto University, Kyoto and CREST/JST, JAPAN

Traditionally, proteins analysis has been conducted under the purified dilute aqueous conditions in most cases. However, it is recently being recognized that structure and functions of natural proteins in live systems are rather different from those under such pure conditions, and thus the protein should be studied in vivo more-details for deep understanding of these biomolecules. For such objectives, development of chemical methods to selectively label, image and regulate a target protein under live cell conditions is now highly desired in the recent chemical biology research. I describe here our recent progress in chemistry-based methods for specific labeling of endogenously expressed proteins driven by coupling of selective molecular recognition and reaction, so-called ligand-directed chemistry (LDchem), under live cell conditions. In LDchem, a reactive and cleavable linker is designed to connect a ligand for selective recognition to a protein-of-interest (POI) with a probe to be tethered to the protein surface. LDchem allows for the protein selective and site selective labeling driven by the proximity effect, in live cells, as well as cell lysates and a pure sample of test tubes. The target proteins are now extended from membrane-bound proteins such as folate receptor, GPCR (G-protein coupled receptors) and neurotransmitter receptors (iGluR, mGluR and GABAR), to several intracellular proteins. In addition, we have very recently proposed a conditional proteomics approach using endogenous protein labeling scheme, by which the fluctuation of Zn proteome is successfully demonstrated in a glial cell line. My group believes and anticipates that such new chemistry may facilitate various aspects of fundamental chemical researches, in addition to progress of basic (neuro) chemical biology, in diagnostic and pharmaceutical applications. I would like to briefly discuss them in my talk.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO1-2**
발표분야: Current Topics on Chemical Biology
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Diversity-Oriented Synthetic Strategy for Developing a Chemical Modulator of Protein–Protein Interaction

박승범

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.

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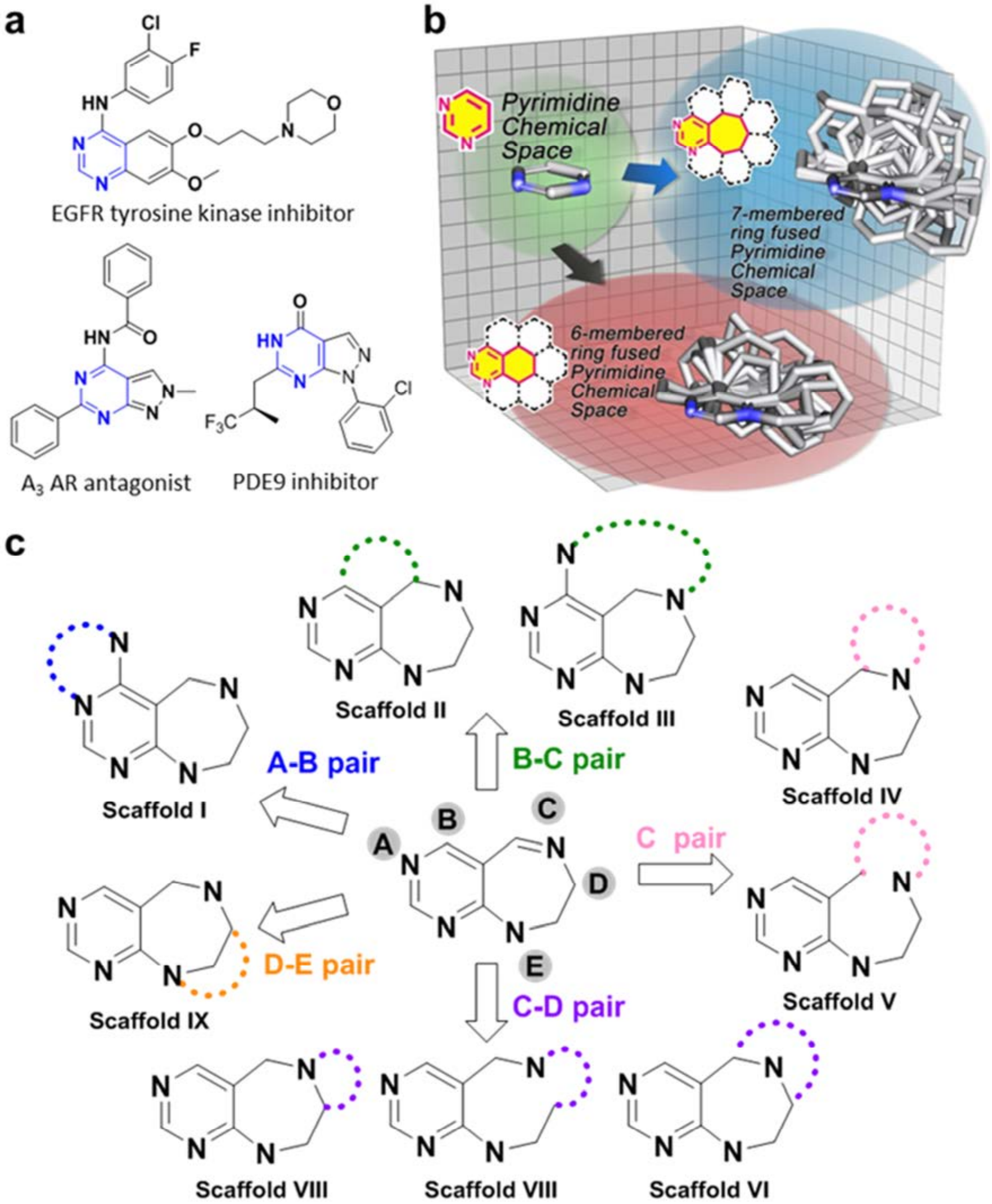
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O
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O
EGFR tyrosine kinase inhibitor
HN
O
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N
N
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A$_3$ AR antagonist
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HN
N
N
N
F$_3$C
Cl
PDE9 inhibitor
b
Pyrimidine Chemical Space
7-membered ring fused Pyrimidine Chemical Space
6-membered ring fused Pyrimidine Chemical Space
c
Scaffold I
Scaffold II
Scaffold III
Scaffold IV
Scaffold V
Scaffold VI
Scaffold VIII
Scaffold VIII
Scaffold IX
A-B pair
B-C pair
C pair
C-D pair
D-E pair
A
B
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발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 기정민

Architecture Mapping of Protein Complexes by Proximity Labeling in Live Cells

이현우

UNIST 화학과

Proximity labeling methods by in situ generated reactive molecules have been developed and has shown remarkable new biological findings which have not been discorved by traditional methods. Our group recently developed an improved method (Spot-ID) by detecting the labeled site generated in proximity labeling using mass spectrometry. This method allows the identification of the labeled protein directly without false positive findings and the structural identification of the labeled protein. Using this method, we could map architercture of the inner mitochondrial membrane (IMM) proteome whose topology at IMM has not been fully characterized yet. Furthermore, this method allowed the identification of unknown elements in the rapamycin-induced interactome on the FK506-rapamycin binding (FRB) domain in living cells. Overall, we have found that sites identified by Spot-ID successfully reflect in vivo structures of protein complexes in living cells.

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Chemical proteomics for host-pathogen interaction study

이준석

한국과학기술연구원(KIST) 분자인지연구센터

Chemical proteomics is an emerging field that utilizes chemical tools to selectively enrich sub-fraction of total proteome. Compared with the conventional proteomic methods, which rely on expression abundance dependent global proteome profiling, chemical proteomics have merits in that engaged proteins can be systematically diversified by structures of chemical tools, and identification & quantitation of low abundant proteins can be also successfully carried out. My group is interested in a development of chemical proteomic tools and method to shed light on molecular mechanism of host-pathogen interaction. Among varieties of infectious pathogens, avian influenza (AI) recently emerged a serious pandemic disease since previously undescribed influenza A virus was identified in 2009. Influenza A viruses are divided into subtypes based on two surface proteins, hemagglutinin (HA, H1-H16) and neuraminidase (NA, N1-N9). Among those subtypes, some strains, such as H5 and H7 viruses, are categorized as highly pathogenic avian influenza (HPAI) viruses and cause high mortality.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO2-1**
발표분야: Biomacromolecules and Protein Engineering
발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 정용원

Nano Cage Protein-based Therapeutics for Cancer Immunotherapy

In-San Kim

Biomedical Research Institute, KIST & KU-KIST School, Korea University

Living creatures have developed diverse bioactive materials with unique structures to survive and adapt to changing environments. Nature in its wonders presents the most intricate and delicate protein structures including cage-like architecture. Perfect and complex symmetry is ubiquitous in protein nanocages and can be engineered for nanomedicines. With respect to the properties of nanocages, I could expect that they may show different biological effects and/or targeting specificity, which can meet the needs of precision medicine as the next generation of DDS and nanomedicine. Particularly, protein nanocages could be developed for the cancer immunotherapeutics.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO2-2**
발표분야: Biomacromolecules and Protein Engineering
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 정용원

Next-generation antibody platform technology

김용성

아주대학교 응용화학생명공학과

The use of monoclonal antibodies (mAbs), which specifically bind to target molecules with high affinity, is of interest for many pharmaceutical and industrial applications. As of January 2017, more than 48 mAbs have been clinically approved in worldwide for diverse indications, mainly cancers and autoimmune/inflammatory diseases. However, the clinical efficacy of mAbs approved for solid-tumor cancer therapy is relatively low as a single agent showing response rates of 8% - 18% even for the qualified patients for particular mAb. Also, market competition becomes very high due to already-marked and coming-soon biosimilar mAbs. Therefore there are great needs for the development of innovative mAbs against new targets and next-generation mAbs with superior profiles to current mAbs. Next-generation antibody will show greater clinical efficacy, reduced side-effects, and more convenient administrations. Further innovative antibody technology which can target cytosolic proteins is required to expand the target space of therapeutic antibodies.In this talk, I will discuss our effort to develop proprietary platform technology for next generation antibody therapeutics, including bispecific antibody, tumor tissue penetrating antibody, and cell-penetrating antibody for targeting of intracellular molecules.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO2-3**

발표분야: Biomacromolecules and Protein Engineering

발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 정용원

FACS-based enzyme engineering for the enhanced production of biomolecules

정기준

KAIST 생명화학공학과

Currently, proteins have indeed found significant applications in various bioprocesses but the full realization of their potential has been limited. To acquire the desired properties, proteins need to be engineered and, for this purpose, directed evolution techniques has been the most powerful tool. Directed evolution consists of an iterative two-step protocol, initially generating molecular diversity by random mutagenesis, then identifying library members with improvements in desired phenotype by screening or selection, and in many cases, the success of directed evolution highly rely on the employed screening strategy. Our research is also focused on the development of efficient strategy for high throughput screening and particularly, we have developed FACS-based high throughput screening in bacterial hosts. In this presentation, I will introduce new screening strategy for the engineering of industrial enzymes towards enhanced production of biomolecules.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO2-4**
발표분야: Biomacromolecules and Protein Engineering
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 정용원

Protein Cage Nanoparticles as Multifunctional Delivery Nanoplatforms

강세병

UNIST 생명과학부

Protein cages, including ferritins, viral capsids, and encapsulins, are biomolecule-based supramolecular polymers and attractive candidates for nano-scale cargo delivery vehicles. While the interior surfaces of the protein cages have been used for encapsulation, attachment and synthesis of organic and inorganic materials, their exterior surfaces have been used for multivalent presentations of molecules, including affinity tags, antibodies, fluorophores, carbohydrates, nucleic acids, and peptides, for molecular targeting and hierarchical structure formation. We genetically and chemically modified various types of protein cage nanoparticles to use them as multifunctional delivery nanoplatforms. Fc binding peptide and domain were genetically inserted onto the surface of protein cage nanoparticles and they formed very stable non-covalent complexes with both human and rabbit IgGs targeting specific cancer cell lines. Protein cage nanoparticles were implemented as intravascular magnetic resonance T1 contrast conjugates via site-selective attachment of Gd(III)-chelateing agents and the potential usage of Gd(III)-chelating agent-conjugated P22 capsids for in vivo MR imaging is validated by visualizing a mouse's intravascular system. We also utilized protein cage nanoparticles as antigen-delivery nanoplatforms, and confirmed their efficacy in inducing DC-mediated antigen-specific immune responses and subsequent melanoma tumor rejection in vivo.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN1-1**
발표분야: Current Trends in Organic Chemistry Ⅰ: Methodology and Application
발표종류: 분과기념강연, 발표일시: 목 13:30, 좌장: 장우동

Design, Synthesis, and Biological Application of Proteomimetics as Protein-Protein Interaction Inhibitors

임현석

POSTECH 화학과

The majority of drugs on the market today target proteins with well-defined small-molecule binding sites, including enzymes. However, some of the most devastating diseases are caused by proteins that do not possess these natural binding sites, such as those involved in protein-protein interactions associated with many cancers. Synthetic molecules capable of inhibiting disease-related protein-protein interactions are thus valuable research tools to investigate molecular functions of target proteins and further could be developed as novel therapeutic candidates. However, discovering such inhibitors is a daunting task due largely to the relatively large and flat protein interfaces involved in protein-protein interactions. In general, typical drug-like small molecules may not be suitable to effectively cover such extended protein contact areas. As such, there is an urgent need for the development of different types of molecules to target protein interfaces. In addition, the shortage of convenient high-throughput screening (HTS) methods is another important reason that makes the identification of such inhibitors so challenging. Here I will present our design and synthesis of novel chemical entities called proteomimetics that are able to mimic protein surface structure and function, allowing them to serve as an excellent source of protein ligands. Moreover, I will also introduce our recent development of simple and efficient HTS methods that enables to facilitate the discovery of chemical inhibitors of many disease-causing protein-protein interactions.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN1-2**
발표분야: Current Trends in Organic Chemistry Ⅰ: Methodology and Application
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 김지민

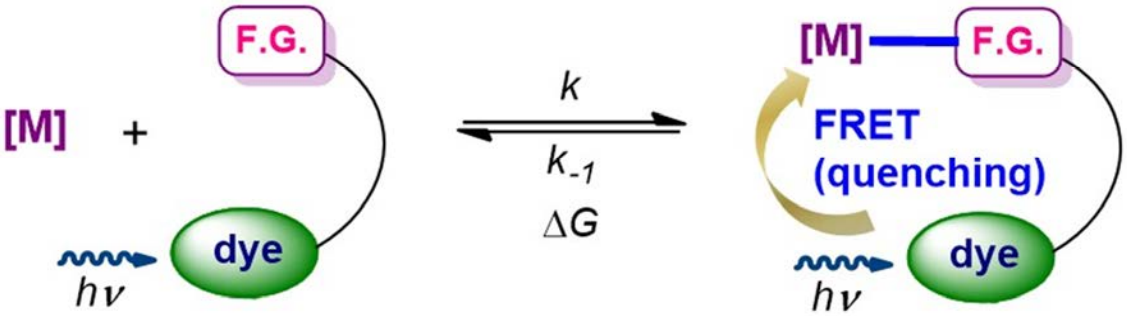
A Guide for Chemoselectivity in Metal-Catalyzed Reactions Involving Multiple Functional Groups

손정훈

충남대학교 화학과

In metal-catalyzed reactions involving multiple functional groups, the functionality preference of a catalyst dictates the identity of the initial adduct or intermediate that can direct the key propagating species and the formation of the final product. With this recognition, we developed a general and direct method using the fluorescence resonance energy transfer (FRET) principle.1 The FRET-based method has been successfully employed to quantify the functionality preference of diverse metal catalysts to their functionalities, such as alkynes, alkenes and allenes. The results enabled us to predict the chemoselectivity in metal catalyzed reactions such as hydroamination reactions of substrates possessing alkyne/alkene, alkyne/allene, or allene/alkene pair, along with answering the mechanistic issues such as the controversial reaction initiation in enyne metathesis. The newly found set of the catalyst-functionality preference might lead to new metal catalysis aided by much clarified reaction mechanisms.

Determination of functionality preference



Quantification

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN1-3**

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

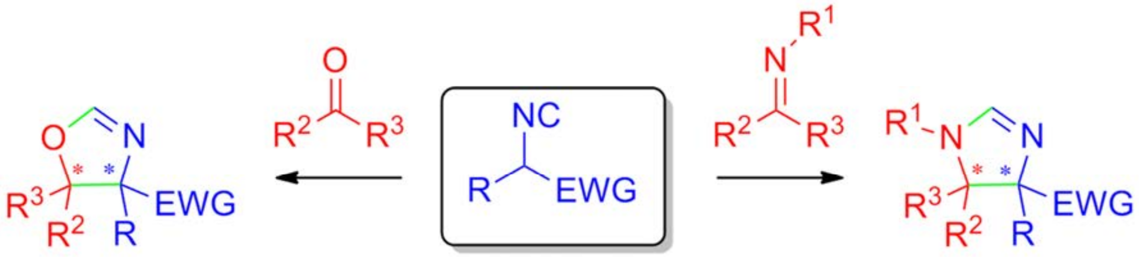
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 김지민

Regio- and Stereoselective Synthetic Transformations of α-Isocyano Compounds

OH KYUNGSOO

중앙대학교 약학대학

With an unusual electronic distribution isocyanides are versatile synthetic precursors in multi-component reactions and metal-catalyzed transformations. The strong σ-donation capability of the carbon atom of isocyanides to metals promotes the corresponding back donation of electrons from the metals to the π* orbital of the isocyanide unit. While such a complexation between isocyanides and metals can promote various coupling reactions, the carbon α to the isocyanide moiety can be also functionalized. Thus, the α-isocyano compounds readily participate in the stereo- and regioselective synthesis of various heterocycles. Previously, our group disclosed the catalytic asymmetric aldol reaction of α-isocyano esters in the presence of cooperative catalyst system of thiourea and chiral Co(I)-Brucine Diol complexes. In addition, we recently explored the click chemistry feature of α-isocyano compounds in the 1,2-bond migration strategy to functionalized pyrroles. With an aim of further extending the chemistry of α-isocyano compounds, we prepared yet unknown α-isocyano compounds and utilized them in the aldol as well as Mannich reactions. In this presentation, we will discuss the stereochemical rationale for the asymmetric aldol and Mannich reactions using α-isocyano compounds.



일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN1-4**

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

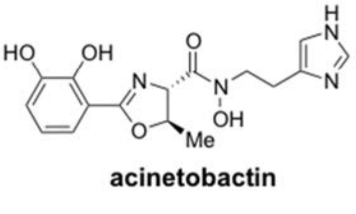
발표종류: 심포지엄, 발표일시: 목 15:00, 좌장: 김지민

Exploitation of the bacterial iron assimilation mechanism for pathogen-specific antibiotic delivery

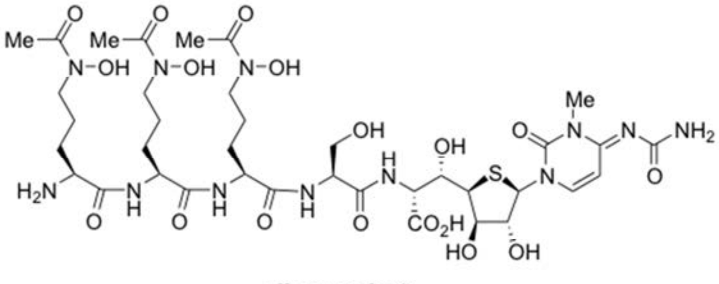
김학중* 송운영 이민욱

고려대학교 화학과

The acquisition of drug resistance by human pathogens is of grave concern to healthcare community, and therefore various novel approaches are being actively pursued worldwide to overcome this threatening problem. The siderophore-antibiotic conjugate (SAC) strategy is a Trojan horse approach, in which the bacterial iron assimilation mechanism based on the utilization of siderophores, small molecule iron chelators, is exploited for intracellular delivery of antibiotic molecules into specific pathogens. The concept of this approach has been well proven by the mode of action of a number of natural product antibiotics possessing the SAC structure, i.e., albomycins and salmycins. However, despite the excellent in vitro, in vivo activity, delivery of those SAC molecules into clinical applications has yet to be limited. In this regard, our laboratory has been interested in addressing a number of pending issues for the design of effective SAC molecules, particularly, in treating drug-resistant Gram-negative pathogens such as *Acinetobacter baumannii*. This presentation will entail our recent progresses in understanding chemistry and biology of acinetobactin, a major siderophore of *A. baumannii*, as well as albomycin δ_2, a prototypical SAC natural product.



acinetobactin



albomycin δ_2

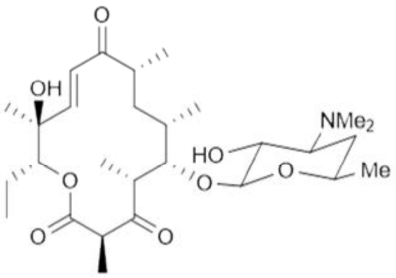
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN1-5**
발표분야: Current Trends in Organic Chemistry Ⅰ: Methodology and Application
발표종류: 심포지엄, 발표일시: 목 15:30, 좌장: 김지민

Utilization of Ring-Closing and Ring-Opening Reactions for the Synthesis of Natural Products

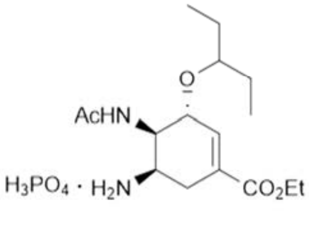
강한영

충북대학교 화학과

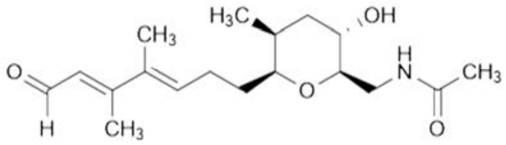
Cyclization is one of the most important types of reactions for the synthesis of cyclic natural products. Macrolide antibiotics are a group of compounds that contains a macrolactone ring to which one or more sugars are attached. Pikromycin is the first isolated macrolide antibiotics before the advent of erythromycin, one of the most renowned macrolide antibiotics. We have exploited successfully the ring-closing metathesis (RCM) reaction for cyclization to secure the framework of this macrolide. Oseltamivir Phosphate (Tamiflu), one of the most typical inhibitors for neuraminidase, contains a six-membered carbocycle. We have also adopted the RCM strategy for the synthesis of oseltamivir phosphate, and have discovered that cis-2,3-bis(hydroxymethyl)aziridine is a good starting material for the synthesis of oseltamivir as well as other nitrogen-containing natural products via ring-opening reactions. The RCM based strategy has also been applied to the stereoselective synthesis of (−)-brevisamide, a monocylic ether amide, containing a characteristic tetrahydropyran ring with an array of substituents. In order to develop more general cyclization strategy for the tetrahydropyran-containing natural products we have investigated the cyclization methods based on the ring opening of epoxides and iodoetherification aiming the synthesis of brevisamide as well as spliceostatin E.



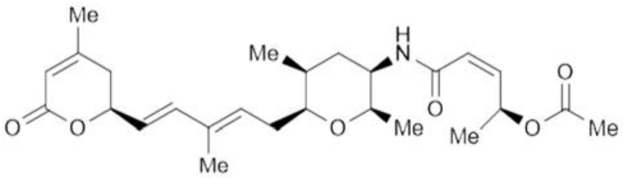
Pikromycin



oseltamivir phosphate
(tamiflu)



Brevisamide



Spliceostatin E

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN2-1**

발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 김영미

Stimuli-responsive Synthetic Chloride Trasporters across Lipid Membranes

정규성

연세대학교 화학과

Ion transport across lipid membranes is a pivotal process in the biological systems. In particular, there have been many different chloride channels that are precisely on and off by biological signals. Dysfunction of these channels causes serious diseases such as cystic fibrosis, Batter's syndrome, Best disease and Myotonia. With hope of potential future use in the treatment of these channelopathies, a large variety of synthetic molecules that can transport chloride ions across lipid and cellular membranes have been studied for the last two decades. We have been focused on the development of small synthetic molecules featuring the controlled activity of chloride transport according to external stimuli such as light and enzymes, which possibly enables delivering the ions in a spatiotemporal manner. Details will be discussed in the presentation

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN2-2**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 김영미

Detection of Heavy Metal Ions and polysaccharides in Aqueous Solution with Fluorescence probes Using Aggregation-Induced Emission process

이건형

인하대학교 화학과

Smart fluorescent probes of which the detection of specific molecules can be controlled are interesting. Fluorescent probes were synthesized by conjugating aggregation-induced emission (AIE) fluorophores with peptide receptors for metal ions and heparins and its contaminant oversulfated chondroitin sulfate (OSCS). The selective detection of dipeptidy probe (1) for specific metal ion in aqueous solutions was controlled by the buffering agents without the change of pH. In phosphate buffered solution, 1 exhibited a selective Off-On response to a soft metal, Hg2+ by 100-fold enhancement of the emission. 1 showed a selective Off-On response to a hard metal, Al3+ in Tris and Hexamine buffered aqueous solution. The detection limits were lower than the maximum allowable level of the metal ions in drinking water by EPA. The fluorescent tripeptidyl probe using an AIE fluorophore exhibited a sensitive turn-on response to heparin, an anticoagulant polysaccharide, in aqueous solution. The probe showed a highly selective response to heparin among biological competitors in human serum samples. Unlike other chemical probes for heparin, the peptidyl probe recognized heparin and then formed nano-sized aggregates, which was potent resistant against heparinase. The dual role of the fluorescent probe for the detection of heparin and inhibition for heparinase made it possible for the selective and sensitive detection of contaminated OSCS in heaprin. This research helps to understand how buffering agents control the selective detection of fluorescent probes using an AIE process for the metal ions in aqueous solutions and the biomedical application of the aggregation process could go far beyond simply sensing.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN2-3**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 10:00, 좌장: 김영미

Ratiometric Two-Photon Probes for Imaging pH Values in Live Samples

김환명

아주대학교 화학과/에너지시스템학과

During the past decade, two-photon microscopy (TPM) has emerged as a powerful tool to imaging studies of biology and medicine. TPM uses two near-infrared (NIR) photons as the excitation source and offers several advantages, including inherent sectioning capability, low photo-damage, longer observation time, and greater tissue penetration depth. To facilitate the use of TPM in biomedical applications, there is a strong need to develop a variety of molecular TP probes for direct, quantitative measurement of target analyte in cell, tissue, and organism level. Recently, we have developed small molecule and emission ratiometric TP probes possessing a significant two-photon brightness, a marked emission color change, easy loading, high photostability, and low cytotoxicity. Intracellular pH varies greatly among individual subcellular compartments. Many metabolic pathways are regulated by pH values. To extend our understanding of the roles of pH in biology and pathology, it is crucial to monitor subcellular pH values and their fluctuation at the cell, tissue, and organism level. In this talk, the design, evaluation, and applications of selected TP probes for pH will be presented.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN2-4**
발표분야: Current Trends in Organic Chemistry Ⅱ: Molecular Recognition
발표종류: 심포지엄, 발표일시: 금 10:25, 좌장: 김영미

A Double Relay: Functional π-Scaffolds Built Upon Resonance-Enhanced Dual Hydrogen Bonds

이동환

서울대학교 화학부

A carbon-based π-conjugation can be functionalized with a hydrogen-bond donor (HBD) group at one end and a hydrogen-bond acceptor (HBA) group at the other end. When such HBD…HBA joint encloses a stable six-membered ring, a synergy between electron delocalization and proton sharing engenders extra thermodynamic stability. Taking this textbook paradigm of resonance-assisted hydrogen bond (RAHB) to the next level, we have recently constructed an extended π-conjugation platform that is embedded with multiple nitrogen-based functional groups to relay two protons in a cooperative fashion. A large shift in charge distribution that accompanies such process can be exploited to tune optical properties. The protons can be replaced with main-group surrogates to produce new fluorophores displaying structure-dependent light-emitting properties over a wide spectral window. In this presentation will be discussed the advent, current progress, and future directions of this chemistry.

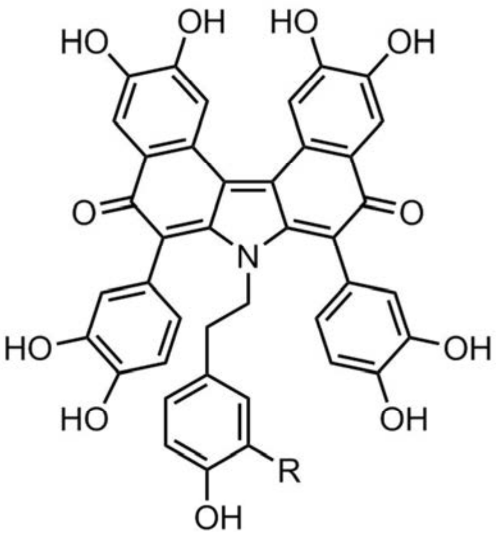
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN3-1**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 천철홍

Tandem [3,3]-sigmatropic rearrangement/cyclization of diaryl hydrazide for the efficient total syntheses of ningalins D and G

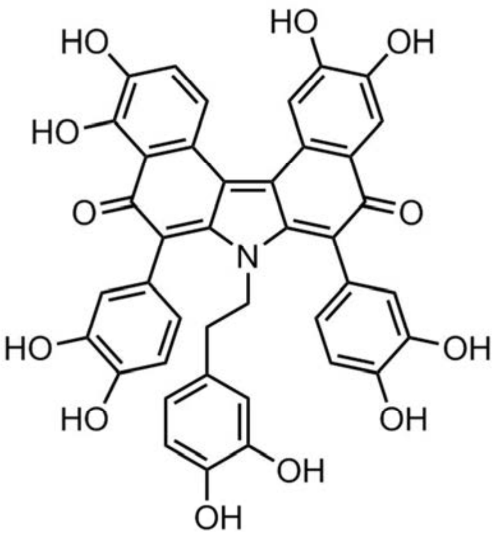
김장엽 조천규*

한양대학교 화학과

Ningalin D is a purple colored benzocarbazole marine alkaloid first isolated by Kang et al. from a western Australian unidentified ascidian belonging to the genus Didemnum. More recently, Capon et al. isolated a closely related marine natural product, named as ningalin G, from the extract of a Southern Australian marine ascidian, Didemnum, and characterized its structure as shown below (Figure 1). As a part of our ongoing investigation on the synthetic utility of aryl hydrazides, we have elaborated a new synthetic route to both ningalin D (1a) and G (2), by way of 7H-dibenzo[c,g]carbazole as the key juncture. Subsequent installation of 3,4-dimethoxyphenyl groups followed by a series of oxidation reactions permitted the total syntheses of the titled marine alkaloids in good overall yields.



1a: R = OH (Ningalin D)
1b: R = H (Purpurone)



2: Ningalin G

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN3-2**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 14:55, 좌장: 천철홍

Copper-Catalyzed C-N Bond Forming Reactions

이윤미

광운대학교 화학과

Amine compounds are important scaffolds in natural products, pharmaceutical targets and functional materials. Among numerous methodologies involving carbon-nitrogen bond forming reactions, a copper catalytic protocol is particularly attractive because copper is relatively cheap, environmentally benign and easy to handle. Recently, our group developed efficient and mild copper-catalyzed systems for C-N bond formation including electrophilic aminations and aza-Michael additions. A variety of heteroaryl amines and enamines are prepared from Cu-catalyzed electrophilic amination of heteroarenes or alkynes using O-benzoyl hydroxylamines as an electrophilic amine source. In addition, β-amino sulfone, β-amino nitrile, and β-amino carbonyl compounds are synthesized through aza-Michael addition of anilines or aza-heterocycles to α,β-unsaturated olefins in the presence of Cu catalyst. The details on the scope of each reaction will be discussed in this presentation.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

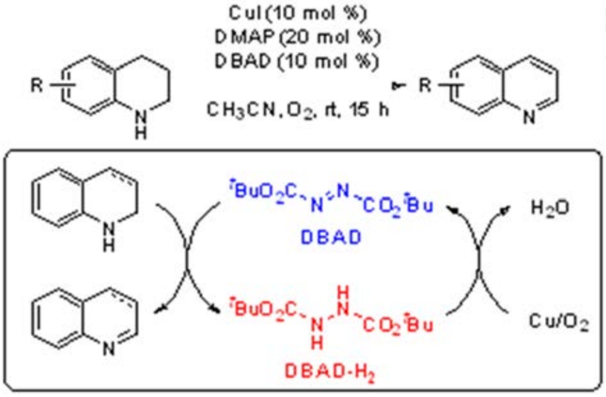
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN3-3**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 천철홍

Catalytic Oxidative Transformations Using Oxygen as a Terminal Oxidant

김진호

인천대학교 화학과

Oxygen is one of the most environment-friendly oxidant, because the oxidation using oxygen produces only water as a by-product. In addition, the oxygen is abundant, easily accessible, and inexpensive compared to other oxidants. Recently, our group developed a co-catalytic system which is consisting of di-*tert*-butyl azodicarboxylate-mediated dehydrogenation of 1,2,3,4-tetrahydroquinoline and aerobic oxidative regeneration of di-*tert*-butyl azodicarboxylate from di-*tert*-butyl hydrazodicarboxylate using molecular oxygen as a terminal oxidant. A variety of quinolines were efficiently synthesized by the developed Cu and di-*tert*-butyl azodicarboxylate co-catalytic system.



일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN3-4**
발표분야: Current Trends in Organic Chemistry Ⅲ: Synthetic Methodology and Catalysis
발표종류: 심포지엄, 발표일시: 금 15:55, 좌장: 천철홍

1,1-Bisborylalkanes: New Types of Organoboron Compounds for the Chemo, and Regioselective Organic Transformations

조승환

POSTECH 화학과

1,1-Bisorganometallic reagents are valuable starting materials for the construction of multifunctionalized molecules. Among them, 1,1-bisborylalkanes, which contain two boryl groups at the same carbon center, are particularly attractive due to their ease of handling, non-toxicity, stability, and propensity to undergo a variety of organic transformations. In this context, our lab is highly interested in the development of regio, chemo and stereoselective organic reactions using 1,1-bisborylalkanes as new types of 1,1-bisorganometallic reagents. In this symposium, the details about our recent findings using 1,1-bisborylalkanes in a range of organic transformations will be presented including 1) an unprecedented transition-metal-free deborylative alkylation of N-heteroaromatic compounds using 1,1-bisborylalkanes as alkyl sources and 2) an unusual chemoselective coupling of 1,1-bisborylalkanes for the transition-metal-free borylation of aryl and vinyl halides.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX

발표코드: **MEDI-1**

발표분야: Recent Trends in Drug Discovery and Technology

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이태호

Versatile strategy for controlling the specificity and activity of engineered T cells

김찬혁

한국과학기술원 생명과학과

Cancer immunotherapy has been drawing growing attention as a novel promising therapeutic modality for cancer. Unlike conventional chemo- or radiotherapy, immunotherapy treats cancer by unleashing the suppressed activity of the patient's own immune system and harnessing its power to fight cancer, to achieve robust anti-tumor responses while minimizing collateral damages to normal tissues. Among several immunotherapeutic approaches, second generation CD19-targeting chimeric antigen receptor (CAR) T cells engineered with costimulatory signaling domains have generated unprecedented anti-leukemic responses in patients with refractory B-cell leukemia. In light of their clinical promise, there has been an explosion of interest in CAR-T cells for cancer immunotherapy, especially for the treatment of relapsed, refractory malignancies. However, the inability to control the activity of this potent "live" drug has resulted in severe treatment related toxicities and the constraint in targeting more than one antigen have limited its general application. In this talk, I will discuss our recent research efforts focusing on addressing these limitations of current CAR-T therapy.

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장소: 일산 KINTEX

발표코드: **MEDI-2**

발표분야: Recent Trends in Drug Discovery and Technology

발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이태호

Discovery of tetrahydroisoquinoline ALK inhibitors and reversible BTK-non-ITK inhibitors

김필호

한국화학연구원 의약화학연구센터

I. Crizotinib (Xalkori by Pfizer) was approved by the US FDA in 2013 to treat anaplastic lymphoma kinase (ALK)-positive non-small-cell lung cancer (NSCLC) patients. The patients treated with crizotinib always relapse usually in one year due to the development of drug resistance. Thus, efforts to develop second-generation ALK inhibitors have been pursued to overcome the drug resistance issues, resulting in development of ceritinib by Novartis and alectinib by Chugai. As our on-going search for ALK inhibitors, we have designed and synthesized derivatives of ceritinib to discover novel ALK inhibitors. Through numerous optimization processes, a pre-clinical candidate (KRCA-605) was discovered. KRCA-605 has a tetrahydroisoquinoline structure, distinct from the existing ALK inhibitors. Biologically, it has far more effective in mouse xenograft studies, compared with ceritinib. Moreover, while ceritinib is not active against G1202R mutant, a crucial crizotinib resistant mutant, KRCA-605 is quite active against G1202R, suggesting that it could circumvent the resistance issues. Activities and ADMETOx profiles of KRCA-605 will be presented.

II. Bruton’s tyrosine kinase (BTK) is a member of the Src-related Tec family cytoplasmic tyrosine kinases playing a crucial role in B cell malignancies. Ibrutinib (Imbruvica), an irreversible BTK inhibitor, was approved for the treatment of mantle cell lymphoma (MCL), chronic lymphocytic leukemia (CLL), and Waldenstrom's macroglobulinemia in 2013-2015, respectively. Although the efficacy of ibrutinib is formidable, the emergence of resistance predominantly from C481 mutations has been observed approximately 65% of CLL patients taking ibrutinib. Moreover, due to the ITK inhibition nature of ibrutinib, combitherapy with immune-checkpoint inhibitors is known to be ineffective. Under these circumstances, the discovery of second-generation BTK inhibitors circumventing resistance and immunocombitherapy issues is in enormous demand. Thus, we have launched a BTK program to discover reversible BTK-non-ITK inhibitors. Compared with ibrutinib, one of our lead compounds exhibited more efficacious results in a murine xenograft model using TMD-8 cells. Current status of the discovery program will be discussed.

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발표분야: Recent Trends in Drug Discovery and Technology
발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 황종연

Multiple Interconnected Pathological Factors in Alzheimer's Disease

임미희

UNIST 자연과학부/화학과

Alzheimer's disease (AD), associated with degeneration of neurons and synapses in the brain, leads to motor impairment and eventual fatality. Neurodegeneration could be related to various interconnected features, including (i) plaque formation from amyloid-β (Aβ) peptide fragments, (ii) metal ion dyshomeostasis and miscompartmentalization, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). The inter-relations between some of these pathological factors have been investigated. Metals are found entangled in the Aβ plaque and likely contribute to Aβ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of Aβ plaque formation. Our understanding of the correlation between these elements and AD neuropathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease.[1] To find a cure for AD, we require a better understanding of the relationship between the various causative factors of this devastating disease. Towards this goal, we need suitable chemical tools capable of targeting and regulating its multiple underlying factors simultaneously.[1,2] Herein, our rational design and preparation of our chemical tools will be discussed with our investigations of their reactivities with targets in vitro as well as their efficacy *in vivo*.[2]References1. *Acc. Chem. Res.* 2014, *47*, 2475-2482; *Chem. Soc. Rev.* 2017, DOI: 10.1039/C6CS00731G.2. *Proc. Natl. Acad. Sci. USA* 2010, *107*, 21990-21995; *Chem. Sci.* 2015, *6*, 1879-1886; *J. Am. Chem. Soc.* 2014, *136*, 299-310; *J. Am. Chem. Soc.* 2015, *137*, 14785-14797; *Nat. Commun*. 2016, *7*, 13115; *J. Am. Chem. Soc.* 2017, DOI: 10.1021/jacs.6b09681.

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장소: 일산 KINTEX
발표코드: **MEDI-4**
발표분야: Recent Trends in Drug Discovery and Technology
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 황종연

GPR119 기전의 당뇨 치료제 개발

양재성

동아제약(주) 신약연구 2팀

당뇨병은 췌장에서 충분한 인슐린을 생산하지 못하거나 신체가 생산하는 인슐린을 효과적으로 사용할 수 없는 경우에 발생하는 만성 질환입니다. 당뇨병은 전 세계적으로 매년 급속한 증가를 보이고 있으며 특히 최근 심혈 관계 질환 관리가 강조되면서 당뇨환자의 지질대사 개선이 강조되고 있다. GPR119 기전의 당뇨 치료제는 기존치료제가 가지고 있는 혈당 강하 뿐 아니라 지질대사 개선을 기대할 수 있는 새로운 기전의 당뇨치료제입니다. DA-441288 은 potent 하고 selective 한 GPR119 agonist 로서 혈당 강하 및 지질 대사 개선 효과를 기대할 수 있는 신약 후보 물질입니다.

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발표코드: **MAT1-1**
발표분야: Nanoscale Structural Analysis of Energy Materials
발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 조성준

In Situ/Operando Neutron/X-ray Scattering for Mechanism Study of Energy Materials

최용남

한국원자력연구원 중성자과학연구부

An *in situ* measurement means a collection of physical or chemical properties of materials at the given sample environments such as temperature, pressure, electric/magnetic field, stress, pH, light and so on. An *in operando* measurement looks similar to the case of *in situ* measurement but is distingushed from that since it was coined as a contineous collection of data under normal working condition (*i.e.* catalytic reaction). Gas (H_2, CH_4, CO_2, etc.) sorption/desorption, structural phase transition, charge/discharge of battery, photosynthetic process, catalytic reactions can be observed in atomic scale by neutron and X-ray scattering experiments. By the virtue of bright X-ray source and high throughput detection technology, time evolving physico-chemical phenomena can be investigated. Especially, neutron can discriminatively probe the behaviors of light elements such as H, Li, C, N, O among heavy elements and thus its application to the energy materials is gradually incresed. Experimental details and results from recent *in situ* and *in operando* neutron/X-ray experiments on hydrogen storage mechanism and catalytic hydrogenation mechanism will be introduced.

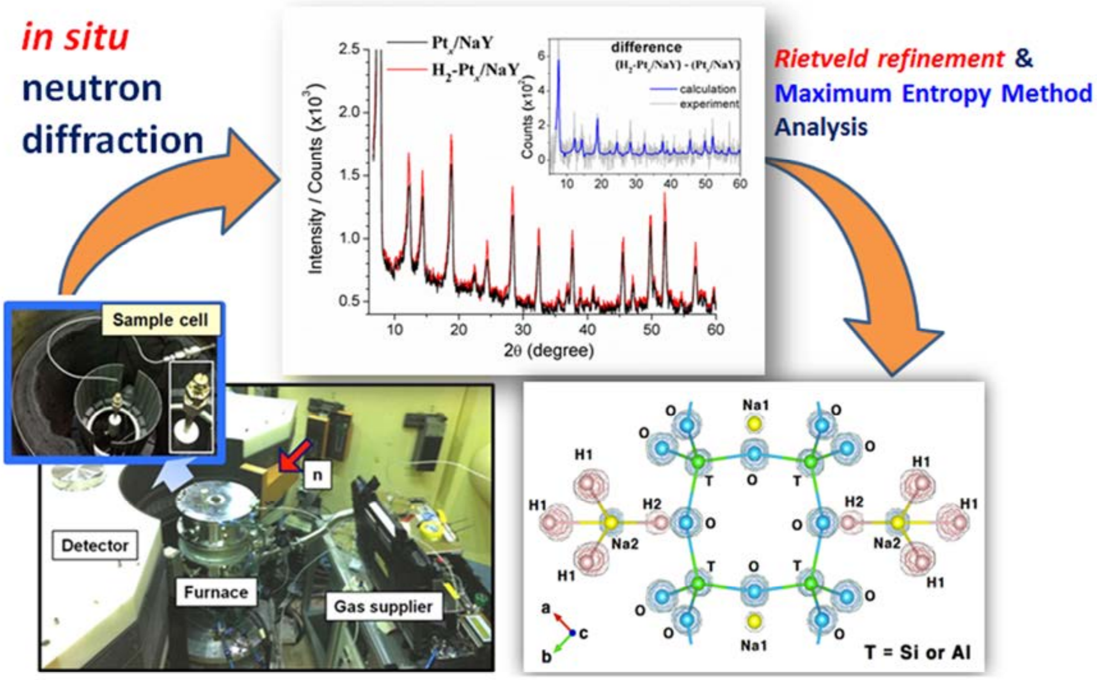

Figure 1. *In situ* neutron diffraction experiment on hydrogen spillover (HRPD@HANARO/KAERI).

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MAT1-2**
발표분야: Nanoscale Structural Analysis of Energy Materials
발표종류: 심포지엄, 발표일시: 금 09:20, 좌장: 조성준

Structure determination from powder X-ray diffraction data and its application to characterization of rechargeable battery electrode materials

홍승태

DGIST 에너지시스템공학

Single crystals are the best forms to analyze their crystal structures in most of cases. However, many of new application materials are available only as powder forms. Electrode materials in battery applications are typical examples, and so are the resultant materials after the electrochemical reactions. If a material adopts an unknown and new structure type and only powder form is available, it would be a great challenge to determine the structure. A method has been developed that is a combination and iteration of the powder and the single crystal refinement techniques. Crystal system and unit cell parameters of a totally unknown structure should be determined first, followed by the space group determination. Structure factors are extracted from the powder data by LeBail fit, that are strongly dependent on the structural model. Because the structure is unknown, the initial model is just a trial one, and thus the extracted structure factors usually include serious errors. However, these are treated as single crystal data, and yet quite useful to get a starting model with a routine single crystal technique. The improved model goes back to be used for LeBail fit, and improved structure factors are extracted. The process is iterated until a complete and satisfactory structure is obtained. Rietveld refinement may be employed in the final step. It should be emphasized that the procedure is not always straightforward, especially for materials with unidentified impurities, high symmetry and/or preferred orientations. In this talk, a recent progress in our exploration for new intercalation chemistry of monovalent and divalent ions into various host materials will be presented, focused on structural determination of new phases during the electrochemical reaction.

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발표코드: **MAT1-3**
발표분야: Nanoscale Structural Analysis of Energy Materials
발표종류: 심포지엄, 발표일시: 금 09:40, 좌장: 조성준

In-situ electrochemical X-ray absorption spectroscopic study of energy conversion nanomaterials

유성종

한국과학기술연구원(KIST) 연료전지센터

A variety of novel composite materials have been used/tested for next-generation energy conversion devices. However, in many cases little is known about their properties and performance, although such fundamental understanding is essential for further advances in energy conversion technologies. Experiments (XRD, XPS, TEM and SEM etc.) may yield many clues to the behavior of those materials, but the interpretations of the local structure of nanomaterials are often controversial due largely to the difficulty of direct characterization. Under such circumstances, X-ray absorption spectroscopic approaches have emerged as one of the most powerful tools for understanding the surface local structure of new energy nanomaterials. This talk will focus on introducing our ongoing efforts in first principles modeling of energy conversion materials. In this talk, I will discuss the properties and performance of Pt(or Pd)-based alloy nanomaterials and composites PEMFCs, particularly the dissolution mechanisms of Pt(or Pd)-based alloy nanomaterials near the surface and interface, with comparisons to those in bulk Pt, as well as the surface and interface effects on the anode an cathode performance, such as oxidation/reduction reaction rate and stability.

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장소: 일산 KINTEX

발표코드: **MAT1-4**

발표분야: Nanoscale Structural Analysis of Energy Materials

발표종류: 심포지엄, 발표일시: 금 10:10, 좌장: 주상훈

Nanostructuring in bulk phases to enhance thermoelectric performance of metal chalcogenide compounds and its structural analysis at the atomic level

이용규 정인*

서울대학교 화학생물공학부

Thermoelectric technology directly converts waste heat into electricity and is considered a promising means of sustainable energy generation. Nanostructuring can effectively scatter heat-carrying phonons to give the significantly reduced lattice thermal conductivity and consequently the enhanced thermoelectric figure of merit (ZT). In this talk, we will discuss about atomic resolution crystal structure of nanostructures embedded in bulk compounds employing aberration-corrected scanning transmission microscopy (Cs-corrected STEM) combined with energy dispersive X-ray spectroscopy and electron energy loss spectroscopy because such nanostructures cannot be analyzed by conventional X-ray diffraction techniques, Afterwards, we will discuss how the nanostructures affect thermoelectric properties of bulk materials.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT1-5**
발표분야: Nanoscale Structural Analysis of Energy Materials
발표종류: 심포지엄, 발표일시: 금 10:30, 좌장: 주상훈

Structural analysis of electrode materials for rechargeable batteries using synchrotron X-ray diffraction

정영화

POSTECH 포항가속기연구소

Powder X-ray diffraction (PXRD) is the most popular and powerful tool to nondestructively characterize the phase of polycrystalline materials under operational conditions. In particular, synchrotron radiation provides high energy and high photon flux, which make it possible to conduct detailed structural analysis of complex materials such as battery electrode materials. I will briefly introduce the 9B HRPD (high resolution powder diffraction) beamline of PLS(Pohang Light Source)-II, and related researches using the HRPD beamline in the first part of the presentation. The second part of this talk will be focused on structural studies of electrode materials for rechargeable Na-ion batteries among various scientific opportunities using synchrotron XRD. Research on Na-based electrode materials has been renewed because of natural abundance and low cost of Na resources. However, structural stability and phase transition behaviors of Na-electrode materials exhibit different trends as compared to the conventional Li-electrode materials. Therefore, both the crystalline structure of an electrode material and its structure changes during electrochemical cycling are considered to be critical factors to understand reaction mechanism of Na-electrode materials. Furthermore, crystal structural information plays a pivotal role to design electrode materials for high performance Na-ion batteries. In this regard, I will present the case study about phase transition behaviors of Na-layered oxides during electrochemical desodiaion/sodiation by in situ synchrotron XRD.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT2-1**
발표분야: Smart Light-Guided Nanomaterials & Devices
발표종류: 심포지엄, 발표일시: 금 14:30, 좌장: 고두현

Properties of Well-Defined Nanostructured TiO2 Prepared from Anodization and Their Application in Energy Devices

박태호

POSTECH 화학공학과

Since first discovery of the titanium element by William Gregor in 1791, the TiO2 has been regarded as one of the most fascinating materials in the various industrial fields due to its distinctive properties. With the advantages including proper electric band position, harmless to human, inertness to chemical, and superior photo-stability make TiO2 an important component in environmental and energy-related applications. In this talk, I will present anodization processes for making advanced one dimensional TiO2 nanomaterials and their electric and catalytic properties.

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장소: 일산 KINTEX

발표코드: **MAT2-2**

발표분야: Smart Light-Guided Nanomaterials & Devices

발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 고두현

Next generation OLEDs for advanced flexibility, transparency and energy efficiency

이정익

한국전자통신연구원 실감소자연구본부

ETRI has reported various research results on OLEDs including flexible OLEDs, transparent OLEDs, OLED lighting and so on since ETRI introduced the first OLED in Korea. Recently, ETRI has carried out projects for advanced flexibility, optical property, and light extraction in OLEDs. We have inestigated on graphene film for transparent pixel electrodes of AMOLED which will reduce the thickness of OLEDs and contribute to the improved flexibility of OLEDs. For reducing reflectance and improving transmittance in OLEDs, we have tried to replace the semi-transparent thin metal top electrode with organic transparent electrodes. Organic nano-lens fabricated by organic vapor phase deposition have been developed to improve light extractions in top emission OLEDs. In this presentation, the detailed results on them will be disclosed.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표분야: Smart Light-Guided Nanomaterials & Devices
발표종류: 심포지엄, 발표일시: 금 15:10, 좌장: 고두현

Light Harvesting Nanomaterials and Devices for the Flexible Photovoltaics: Dye-Sensitized and Perovskite Solar Cells

고민재

한양대학교 화학공학과

There have been significant progresses in the dye-sensitized (DSSCs) and perovskite solar cells (PSCs). Further cost reduction in high-speed manufacturing can be accomplished by continuous roll-to-roll printing processes using a flexible plastic substrate. Lightweight and flexible plastic solar cells can be installed even on non-flat surface, which makes them a possible ubiquitous power source for mobile electronics. To fully utilize these kinds of advantages in DSSCs and PSCs, mechanical durability as well high efficiency should be guaranteed. In this talk, we will introduce several strategies to address these issues using new nanomaterials and novel architectures.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표코드: **MAT2-4**
발표분야: Smart Light-Guided Nanomaterials & Devices
발표종류: 심포지엄, 발표일시: 금 15:30, 좌장: 고두현

Liquid crystal materials in the nanoconfinement and its optical applications

윤동기

KAIST 나노과학기술대학원

Liquid crystal (LC) material is now everyday substance on hand and the wall at home. This big success is based on the well-controlled LC domain in large area, now extending to the various kinds of applications beyond display applications, for example, organic semiconductors, optical devices and patterning applications. A key technique to realize these applications is the orientation control of LC phases over large areas with external efforts such as applying external electric or magnetic field, topographic confinement and mechanical shearing method.

Here, we used porous anodic aluminium oxide (AAO) film to control the nanometer-scaled structures of low molecular weight LC materials.[1-4] There have been many efforts to see the structural behaviours of LC phases in porous AAO film, including high-resolution calorimeter, deuteron nuclear magnetic resonance (2H-NMR) and dielectric relaxation spectroscopies. Although these techniques provide the information of the molecular dynamics for the orientation and the phase transition, they could not show the direct clues, indeed additional efforts should be used to analyse the data. However, grazing incidence X-ray diffraction (GIXD) technique can directly reveal the molecular ordering and orientation of LC phases in the nanoconfined geometry when this is used with a 2D CCD camera, directly showing the in-plane and out-of-plane information of the molecular behavior of LCs. We have controlled the molecular orientation of nematic (N) and smectic A (SmA) liquid crystal (LC) phase in chemically modified porous AAO film. The nano-templated LC could show the adjustable optical and photonic characteristics.[5,6]

References:
[1] H. Kim *et al*, *Proc. Natl. Acad. Sci. U.S.A*, **111**, 14342 (2014)
[2] S. Lee, *et al*, *Soft Matter*, **11**, 3653 (2015)

[3] S. Lee, *et al*, *Langmuir*, **31**, 8156 (2015)

[4] H. Kim *et al*, *Science Advances*, **3**, e1602102 (2017)

[5] S. H. Ryu *et al*, *ACS. Appl. Mater. Interface*s, **9**, 3186 (2017)

[6] S. H. Ryu *et al*, *ACS Appl. Mater. Interfaces*, **8**, 17707 (2016)

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT2-5**
발표분야: Smart Light-Guided Nanomaterials & Devices
발표종류: 심포지엄, 발표일시: 금 15:50, 좌장: 고두현

Highly efficient organic-inorganic hybrid perovskite light-emitting diodes by surface engineering

송명훈

UNIST 신소재공학부

The use of hybrid organic-inorganic perovskites in optoelectronic applications are attracting an interest because of their outstanding characteristics, which enable a remarkable enhancement of device efficiency. Here, we demonstrate highly efficient perovskite lgiht-emitting diodes by surface treatment to passivate the defect sites of methyl ammonium lead tribromide (MAPbBr3) with uniform morphology. This treatment greatly enhanced PeLEDs efficiency, with an improved external quantum efficiency (EQE), enhanced photoluminescence (PL), a lower threshold for amplified spontaneous emission (ASE), a longer PL lifetime and enhanced device stability.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT2-6**
발표분야: Smart Light-Guided Nanomaterials & Devices
발표종류: 심포지엄, 발표일시: 금 16:10, 좌장: 고두현

Light Harvesting Polymeric Chromophore-Catalyst Assemblies for Photoelectrochemical Water Splitting Devices

Gyu Leem* **Kirk S Schanze***

University of Texas at San Antonio

Dye-sensitized photoelectrochemical cells (DSPECs) convert energy from the sun directly into fuel. The DSPEC approach is a hybrid based on molecular light absorption and excited state electron or hole injection into the conduction or valence bands of high band gap semiconductors. Toward fabricating DSPEC devices, we have reported a Layer-by-Layer (LbL) self-assembly process to construct polychromophore–catalyst assemblies consisting of a cationic polymer-based Ru polychromophores and water oxidation catalyst or proton reduction catalyst. The photophysical and electrochemical properties of the polychromophore-catalyst assembly were characterized in solution and at the semiconductor interface and the energy/electron transfer processes were investigated in the polymer assembly. Importantly, photocurrent measurements of the polyelectrolyte LbL films formed on mesoporous semiconductor substrates demonstrate a clear anodic photocurrent response, coupled with the observation of O2. This is the first report to demonstrate the use of polyelectrolyte LbL to construct chromophore–catalyst assemblies for water splitting reaction.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC1-1**

발표분야: Recent Trends in Electrochemistry I

발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 석정돈

Electrochemical Generation of Single Emulsion Droplets and in-situ Observation of Collisions on an Ultramicroelectrode

<u>장진호</u>

성신여자대학교 화학과

The Br−/Br2 redox couple in aqueous solution has been often employed for redox flow batteries along with N-methyl-N-ethyl pyrrolidinium bromide (MEPBr) as a bromine-complexing agent, which forms insoluble organic droplets of MEPBr3 complexes during electro-oxidation of Br−. We, for the first time, report the electro- chemistry of Br− electro-oxidation in electrochemically generated single droplets of MEPBr3 using the current transient method on an ultramicroelectrode (UME). Current spikes were observed in the chronoamperogram of the aqueous solutions containing more than 32 mM of MEPBr, and they correspond to electro-oxidation of Br− in MEPBr3. The voltammetric behavior of Br− electro-oxidation in single droplets of MEPBr3 was similar to that in the aqueous phase. The maximum concentration of Br− in the MEPBr3 droplets was estimated to be ～7.5 M by fitting the observed current transient curves to the simulation using a bulk electrolysis model. Our study reveals that MEPBr3 also plays a vital role as an electrochemical reaction medium for Br− electro-oxidation in the Br−/Br2 redox system.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC1-2**

발표분야: Recent Trends in Electrochemistry I

발표종류: 심포지엄, 발표일시: 목 13:55, 좌장: 석정돈

Electrochemical imaging of single nanostructured electrocatalyst

김양래

광운대학교 화학과

Two unique carbon nanostructures, graphite nanostrands and modified graphite nanoblisters have been observed at the surface of highly oriented pyrolytic graphite and activated for hydrogen evolution reaction in sulfuric acid solution by electrochemical methods with high spatial resolution, respectively. The entire substrate has been investigated by electrochemical techniques through voltammetric scanning electrochemical cell microscopy as well as complementary microscopy techniques such as scanning electron microscopy, atomic force microscopy, and micro-Raman.

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장소: 일산 KINTEX
발표코드: **ELEC1-3**
발표분야: Recent Trends in Electrochemistry I
발표종류: 심포지엄, 발표일시: 목 14:20, 좌장: 석정돈

Conditioning-free magnesium chloride-complex electrolyte for rechargeable magnesium batteries

오시형

한국과학기술연구원(KIST) 에너지융합연구단

The development of new battery systems beyond Li-ion is a hot topic world-wide, reflecting a rapidly expanding market for EVs and commercial large-scale ESS for load-leveling or emergency backup power. Rechargeable magnesium batteries have been proposed as a promising alternative to Li-ion since as a negative electrode material, magnesium has a high gravimetric and volumetric capacity and a low standard reduction potential of -2.372 V. Furthermore, magnesium is naturally abundant in the earth’s crust and thus magnesium batteries can be potentially manufactured at lower cost. One of the most critical challenges for this system is development of an electrolyte system which possesses a wide electrochemical window, while maintaining reversibility for Mg plating-stripping on the negative electrode. Recently, Aurbach et al. proposed a highly stable electrolyte called MACC, which consists of all inorganic species and is stable over 3.0 V. Although the precise nature of speciation is yet undefined, this electrolyte needs a complex activation process called ‘electrolytic conditioning’ involving up to a hundred cycles before use. We report a MACC-related electrolyte which does not require this complex electrolytic conditioning. Its simple one-pot synthesis was accomplished by the dissolution of magnesium metal in AlCl3/THF solution using CrCl3 as a promoter. We further demonstrate that this electrolyte functions well in the prototype cell consisting of Mo6S8 and Mg as positive and negative electrode, respectively. We also show that the employment of an ionic-liquid co-additive further extends the stability window. The crucial advantage originates from the very high Mg to Al ratio in the new electrolyte “MaCC”, which promotes 100% coulombic efficiency for Mg in the first cycle.

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발표분야: Recent Trends in Electrochemistry I
발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: 석정돈

Real-time & Quantitative Analysis of Li-air Battery Materials by In-situ Differential Electrochemical Mass Spectrometry

김동욱

한국화학연구원 차세대전지소재연구센터

Lithium-air battery is a promising battery technology for next generation battery for a long-driving-range electric vehicle. However recent tremendous research studies have found that there are many issues such as fast capacity fading on cycling, high overpotential in charge, low oxygen efficiency, etc. Since the problems are largely due to instability in the electrolytes and electrodes, many researches are driven to develop stable materials for electrolytes and electrode for true rechargeable lithium-air battery. During the cycles, the reactive superoxide ion and lithium peroxide may attack the susceptible organic electrolyte and carbon cathode, yielding several by-products such as lithium carbonate, lithium carboxylate, and lithium alkyl carboxylates. The side-products caused evolution of carbon dioxide instead of oxygen in charge, loss of capacity, and finally failure of the cell operation. Many research groups are attempting to develop a stable electrolyte and cathode to suppress the side reaction in the cell. To identify stable materials, they measure mainly coulomb efficiency, energy efficiency, and cyclability. There is another important parameter to be evaluated in the lithium air cell: oxygen efficiency, which is a ratio of oxygen consumed in discharge to oxygen re-generated in charge stage. In-situ differential electrochemical mass spectrometer (DEMS) is a useful instrument to measure the oxygen efficiency. It is composed of an electrochemical cell connected with a potentiostat and a mass spectrometer, to measure a gas product generated during an electrochemical reaction in the cell in in-situ and real-time mode. In this talk, I will present and discuss how to utilize in-situ DEMS for identifying and developing stable lithium-air battery materials.

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발표분야: Recent Trends in Electrochemistry I
발표종류: 심포지엄, 발표일시: 목 15:10, 좌장: 석정돈

공액 고분자를 기반으로 하는 유기 및 복합 열전소재

장광석

한경대학교 화학공학과

폐열로부터 전기에너지를 얻어낼 수 있는 열전소재에 관한 관심이 점점 증가하고 있다. 일반적으로 높은 Seebeck 계수와 높은 전기전도도, 낮은 열전도도를 가지는 소재가 좋은 열전소재로 인식되고 있다. 최근에는 유기 열전소재 분야의 연구가 활발히 진행되고 있다. 유기 열전소재는 아직까지 무기 열전소재에 비해 성능이 매우 떨어지지만, 유연하고 다양한 공정 적용이 가능하다는 장점이 있다. 유기 열전소재의 성능을 향상시키기 위해서 공액 고분자의 도핑을 최적화하거나 CNT 와 같은 나노카본을 복합화하는 연구가 활발히 진행되고 있다. 본 발표에서는 공액 고분자를 기반으로하는 유기 열전소재와 CNT/공액 고분자 복합 열전소재를 소개하고, 열전소재와 열전소자 제작에 관련된 공정들을 소개하고자 한다.

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장소: 일산 KINTEX

발표코드: **ELEC2-1**

발표분야: Recent Trends in Electrochemistry Ⅱ

발표종류: 심포지엄, 발표일시: 금 09:00, 좌장: 오일환

Use of Dendrimers for Amplified Electrochemiluminescence

김주훈

경희대학교 화학과

Electrochemiluminescence (ECL) provides beneficial characteristics over photoluminescence, including low background emission, good temporal and spatial controllability, robustness, and instrumental simplicity. Thus, the ECL technique has been utilized as a versatile tool in a variety of analytical applications. To further expand the usefulness of ECL in analytical applications, many promising approaches have been suggested for amplification of ECL signals. Of the approaches, we recently reported the use of amine-terminated polyamidoamine (PAMAM) dendrimers for the enhancement of ECL. In the present talk, we discuss the recent reports about the use of dendrimers for enhanced ECL. First, we discuss highly enhanced ECL of $Ru(bpy)_3^{2+}$ (bpy = 2,2'-bipyridyl) or luminol with appropriate coreactants on electrodes modified with amine-terminated dendrimers encapsulating catalytic nanoparticles [1-3]. Second, we discuss intense ECL of $Ru(bpy)_3^{2+}$ in the presence of amine-terminated dendrimers as a coreactant [4].[1] Jihye Kwon, Seo Kyoung Park, Yongwoon Lee, Je Seung Lee, and Joohoon Kim, Biosens. Bioelectron., 2017, 87, 89-95.[2] Jisoo Yoon, Taehoon Cho, Hyojung Lim, and Joohoon Kim, Anal. Bioanal. Chem., 2016, 408, 7165-7172.[3] Soon Bo Lee, Jihye Kwon, and Joohoon Kim, Electroanalysis, 2015, 27, 2180-2186.[4] Yeoju Kim and Joohoon Kim, Anal. Chem., 2014, 86, 1654-1660.[5] Soon Bo Lee, Youngwon Ju, Yeoju Kim, Chong Min Koo, and Joohoon Kim, Chem. Commun., 2013, 49, 8913-8915.[6] Hyein Lee and Joohoon Kim, ChemElectroChem, 2017, Under revision.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
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발표분야: Recent Trends in Electrochemistry Ⅱ
발표종류: 심포지엄, 발표일시: 금 09:25, 좌장: 오일환

Electrochemical SERS Investigation of Formic Acid Electrooxidation on Pt Modified Au Surfaces

김종원

충북대학교 화학과

The electrooxidation of formic acid (FA) on Pt has received great attention because of its fundamental significance as a model reaction and its technical importance in fuel cells. In this work, the mechanism of FA electrooxidation on Pt modified Au surfaces was investigated via in situ electrochemical surface-enhanced Raman scattering (SERS). SERS-active DAR@Pt(n) substrates were prepared using the self-terminating electrodeposition of Pt on dendritic Au rod (DAR) surfaces, wherein the amount and coverage of Pt were precisely controlled by applying a different number of potential steps (n) during the electrodeposition process. The electrocatalytic activity of FA was highly dependent on the Pt coverage and thickness on DAR@Pt(n), which was investigated by electrochemical SERS. The amount of CO produced by the dehydration of FA, the potential-dependent SERS intensity variation, and the Stark slopes were examined on different DAR@Pt(n) surfaces. Based on these results, insights into the mechanistic interpretation of FA electrooxidation on Pt-Au system are discussed.

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일시: 2017년 4월 19~21일(수~금) 3일간

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발표코드: **ELEC2-3**

발표분야: Recent Trends in Electrochemistry Ⅱ

발표종류: 심포지엄, 발표일시: 금 09:50, 좌장: 오일환

High-Voltage Battery Interfaces

송승완

충남대학교 응용화학공학과

Increasing the energy density of Li-ion batteries is crucial for the success of electric vehicles and grid-based energy storage. One of the promising approaches is to increase the capacity of cathode material such as Li-rich layered oxide by increasing the charge cut-off voltage above 4.5 V vs. Li/Li+. The anodic instability of conventional electrolyte however limits its charging to high-voltages. Overcoming this issue relies on electrolyte breakthrough and the stabilization of interfaces of both cathode and anode in a high-voltage battery. In this talk, I will introduce our recent research results on the high-voltage interfacial phenomena of Li-rich layered oxide cathode and graphite anode in a Li-ion full-cell, and their stabilization with high-voltage electrolyte.This work was supported by the Korean Ministry of Trade, Industry & Energy (R0004645).

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발표분야: Recent Trends in Electrochemistry Ⅱ
발표종류: 심포지엄, 발표일시: 금 10:15, 좌장: 오일환

General overview of semiconductor composite for photoelectrochemical water splitting

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. Composite structures, typically comprising a primary photon absorbing semiconductor with a secondary material 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 interface. These composite structures are divided into four different configurations depending on the possible electron-hole separation mechanism. Typically, the synthesis and characterization of the semiconductor electrodes and the effect of co-catalyst layers on the PEC performance are discussed in detail.

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Phantom Catalysis of Ni^{2+} for Water Oxidation in Neutral Condition: Electrochemical Identification of its Heterogeneity and the Combination with Photoelectrode

조성기

금오공과대학교 에너지화학공학과

본 연구에서는, 다양한 전기화학분석법을 이용하여 중성용액에서의 Ni2+ 이온에 의한 전기화학적 물산화 촉매 반응을 연구하였다. Scanning Electrochemical Microscope 을 이용한 산소 발생 관찰을 통해, phosphate buffer 용액에서 Ni2+ 이온이 물산화 반응을 촉진하는 것을 확인하였다. 본 전기화학적 촉매 작용은, 물질 확산이 촉매 반응에 관여하고, 전극 표면에 촉매층이 형성되지 않는 등, homogeneous catalysis 의 특성을 나타내나, 전기화학분석을 통해 촉매 특성이 heterogeneous catalysis 임을 확인할 수 있었다. Cyclic voltammetry, coulombic titration, electrochemical quartz microbalance 분석을 통해, 전극 표면에 4 nm 이하의 촉매층 (Ni-Pi) 이 형성되는 것을 확인할 수 있었다. 다양한 전압 및 pH 에서의 Ni-Pi 촉매층의 형성 및 그 특성을 분석한 결과, 촉매층은 전압이 인가되는 경우에만 전극상 존재하는 것을 확인할 수 있었으며, 이로 미루어 Ni-Pi 촉매는 Ni(III) oxide 로 구성되어 있고, 이의 산화반응이 전기화학적, 화학적으로 비가역적임을 추정할 수 있었다. 또한 Ni-Pi 촉매반응은 heterogeneous catalysis 임에도 불구하고, phosphate ion 의 농도와 확산이 관여함을 알 수 있었다. Ni2+ 의 전기화학적 촉매 특성은 타 촉매에 비해 뛰어나진 않았으나, 광전극과 결합하였을 경우 매우 우수한 특성을 나타내었으며, 산화물 광음극과의 synergetic effect 에 대해서도 확인하였다.

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초등 화학에서의 물질 개념

임희준

경인교육대학교 과학교육과

화학은 물질에 관한 학문이며, 학교 과학교육에서 화학 학습의 시작은 물질에 대하여 배우는 것으로 출발한다. 초등학교 과학(화학 영역)에서는 전통적으로 물질의 의미와 성질, 혼합물의 분리, 물질이 상태 등이 지도되어 왔는데, 각 단원에서의 물질의 의미가 약간 상이하게 다루어지고 있다. 이에 초등 화학에서 지도할 물질의 개념과 범위, 방법 등에 대하여 고찰해보고자 한다. 이를 위해 외국 교과서와 우리나라 6 차 이후의 교육과정과 교과서 등을 비교 검토하여 물질의 의미가 어떻게 다루어지고 있는지 비교하고, 초등 화학에서의 물질 개념에 대한 교과서 저자와 현장 교사의 인식을 살펴보았다. 이를 통해 초등에서 다루는 물질 개념을 정리해보고자 한다.

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중학교 화학에서 물질 개념

백성혜

한국교원대학교 화학교육과

화학은 물질을 다루는 학문이다. 그러나 물질을 정의한다는 것은 매우 복잡한 일이다. 물질을 물체와 대조하여 설명하는 방식은 오랜 전통이었으나, 이러한 설명의 비효율성과 교육적 혼란은 지속적으로 문제가 제기되어 왔다. 또한 물질을 순물질로 재정의하는 문제에 대한 합의도 아직까지 이루어지지 못하였다. 따라서 물질의 세가지 상태를 거론할 때, 고체, 액체, 기체가 과연 물질인지 물체인지에 대한 논의가 꾸준히 거론되어 왔다. 이번 심포지움에서 연구자는 이러한 교육적 혼란을 바로잡기 위한 화학교육학자들의 관심을 촉구하기 위한 제안을 하고자 한다.

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화학 교과과정에서 토론이 지니는 성찰적 의의에 대한 고찰

남창훈

DGIST 융복합대학 기초학부

교과과정에서의 성찰은 교과과정에서 이뤄지는 강의와 여러 활동을 통해 교과에서 다뤄진 여러 정보를 분석하고 종합한 다음 이를 적용한 후, 그 결과를 공유하면서 발전 또는 확장된 생각할 요소들과 문제의식을 발견하는 과정을 아울러 지칭한다. 교과과정에서 이러한 성찰이 지니는 의의에 대해 많은 논의가 이뤄졌고, 일반적인 차원에서는 그 중요성이 대체로 동의 되고 있다. 그러함에도 일반화학을 비롯한 기초과학 교과과정에서 성찰이 최상위의 교과 목표로 설정되고 있는지에 대해서는 의문의 여지가 있다. 보통 기초과학의 필수적인 지식 정보의 체계적 수용과정으로 대학 일학년 교과과정을 자리매김하는 것이 현실이기 때문이다. 4 차 산업혁명 시대를 맞이하고 있는 현재 상황에서 성찰이 지니는 중요성을 다시 상기시킴으로써 이러한 현실을 어떻게 타개해 나가야 할지 총론을 통해 논의하고자 한다. 구체적으로는 일학년 화학 교과에서 토론을 통해 수행되는 성찰 과정의 구체적인 사례를 공유하고 그 의의에 대해 논의하고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR-1**
발표분야: Current Trends in Chemistry for Water Science and Technology
발표종류: 심포지엄, 발표일시: 목 13:35, 좌장: 이윤호

Investigation into persulfate activation mechanism: Radical-induced oxidation pathway versus electron-transfer mediating pathway

이재상

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수산화라디칼의 강력한 산화력에 기반하는 고도산화공정을 대체하기 위한 노력으로서, 최근 과황산염을 황산라디칼의 전구체로 활용하는 소위 과황산염 활성화 (persulfate activation) 공정에 대한 연구가 활발히 진행되고 있다. 황산라디칼은 수산화라디칼에 비견되는 고활성 산화종으로서 상이한 유기오염물질의 산화분해를 가능케 하며, 과황산염은 과산화수소 (수산화라디칼 전구체) 대비 고상으로 합성이 가능하고 다양한 활성화 기법을 통해 효율적인 라디칼로의 전환이 용이하다. 과황산염 활성화를 위해 널리 활용되어 온 활성화제는 코발트나 망간과 같은 전이금속계열의 물질로서 일전자전달반응을 (one-electron transfer) 통해 과황산염을 환원시킴으로써 황산라디칼을 생성하는 것으로 알려져 있다. 반면, 최근 탄소계열 혹은 금속산화물계열 활성화제의 경우 라디칼이 관여하지 않는 비라디칼 메커니즘에 의한 과황산염의 활성화에 대한 실험적 증거가 다수 보고되고 있다. 본 발표에서는 여러 종의 금속계열 및 탄소계열 활성화제를 활용한 과황산염 활성화 메커니즘을 다양한 실험 기법을 (예: 라디칼 소모제 (radical quencher) 효과, 산화부산물 분석, 기질특이성, 형성전류량 변이, 전자스핀공명법) 통해 고찰하고, 그 결과로부터 활성화제 선택에 따라 오염물질의 산화분해 메커니즘이 상이하게 이루어짐을 제시할 것이다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR-2**
발표분야: Current Trends in Chemistry for Water Science and Technology
발표종류: 심포지엄, 발표일시: 목 14:00, 좌장: 이윤호

Development of a sustainable treatment technology for oxyanions in drinking water

CHOE JONG KWON

서울대학교 건설환경공학부

Providing safe drinking water to the public is a demanding challenge. Depletion of pristine freshwater resources in many parts of the world leads to the use of anthropogenically-impaired water sources, requiring intensive treatment of contaminants. While treatment of these waters is often technically feasible, best available technologies often impose a high financial, environmental, and social cost. A key challenge is developing new water treatment technologies that are more sustainable. A prime example is ion exchange, the go to technology for oxyanions (e.g., perchlorate, nitrate) in drinking water. While effective, this technology suffers from high costs associated with salt use for once-used regeneration brine, and high environmental impacts related to salt mining and waste brine disposal. I will present my research on developing a new sustainable treatment technology for removing the oxyanions, nitrate and perchlorate, from drinking water. The new technology relies on supported Pd-based catalysts to convert oxyanions via reduction by hydrogen to harmless end products. It can be used to directly remove nitrate and perchlorate from drinking water, or in combination with ion exchange to treat waste brine and enable its reuse for resin regeneration. Mechanisms of perchlorate reduction are evaluated by combining kinetic studies with x-ray characterization. The kinetic results are used to design a reactor, and environmental impacts of catalytic treatment are compared to alternative treatment technologies (i.e., ion exchange, biological treatment) using a life cycle assessment tool. The results identify key weaknesses in each technology that impact sustainability, and motivate basic research on improving the activity and longevity of the supported catalysts.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR-3**
발표분야: Current Trends in Chemistry for Water Science and Technology
발표종류: 심포지엄, 발표일시: 목 14:30, 좌장: 조민

Upconversion: mechanism and application to energy and environemtal engineering

김재혁

부산대학교 환경공학과

광에너지 상향기술(Upconversion)은 낮은 주파수를 가지는 두 개 혹은 그 이상의 광자를 이용해 높은 주파수를 가지는 하나의 광자를 생산해내는 기술로 정의된다. 일반적인 형광·인광 현상이 Stokes-emission 을 발생시킴에 반해, anti-Stokes emission 을 발생시키는 Upconversion 물질의 독특한 광학적 특성은 태양광에서 큰 비중을 차지하지만 낮은 광자에너지 탓에 활용되지 못했던 가시광선 및 근적외선 영역의 광자를 고에너지의 광자로 전환시킴으로써 태양전지 및 광촉매 등 광학에 기반을 둔 기기의 효율을 획기적으로 향상시킬 수 있는 신개념 에너지 변환기술로 평가받고 있다. 특히 삼중항-삼중항 소멸(Triplet-Triplet Annihilation, TTA)에 의한 Upconversion(이하 TTA-UC)은 국내에는 산·학을 통틀어 연구보고사례가 전무할 정도로 생소한 연구분야지만 높은 양자 수득률, 넓은 흡광영역, 태양광 직접활용 등의 탁월한 장점들이 최근 잇따라 학계에 보고되며 2000 년대 후반부터 신개념 광에너지 변환기술의 최대 화두로 떠오르고 있다. 광학기기(광촉매 등)를 광활성화시키지 못하고 소실되는 밴드갭 이하의 광에너지를 응축하여 활용가능한 고에너지로 변환시키는 TTA-UC 는 공정 자체가 매우 단순하면서도 직관적이며 수질/대기환경 분야에 광범위하게 이용되고 있는 광촉매 관련 연구분야 뿐 아니라 태양전지, 수소생산 등 신재생 에너지 분야에 직접 활용가능한 기술이라 할 수 있다. 본 연구발표에서는 아직 국내학계에 생소한 연구분야인 TTA-UC 기술의 기본원리를 소개하고 현 기술개발 단계(State-of-art)와 차기 환경-에너지 공학에의 응용가능분야를 짚어본다. 또한 실제로 본 연구실에서 개발된 다양한 Upconversion 물질의 제조법과 광학적 특성을 소개·분석하고, Sub-bandgap 에너지의 광자 조사시에 수계에서 일어나는 Upconversion 현상에 의해 광촉매가 광활성화된 연구결과를 소개한다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ENVR-4**

발표분야: Current Trends in Chemistry for Water Science and Technology

발표종류: 심포지엄, 발표일시: 목 14:55, 좌장: 조민

전기화학 기반 하폐수 중 암모니아성 질소 제어를 위한 반응 동역학 모델 및 촉매 양극 개발

조강우

POSTECH 환경공학부

최근 하수고도처리 기술의 광범위한 보급에도 불구하고 환경기준의 지속적인 강화로 총질소 기준 국내 호소의 좋은물과 매우나쁨 비율은 1992 년 각각 2%와 20%에서 2012 년 0%와 65%로 지속적인 총질소 처리 기술의 개발 및 보급이 필요한 것으로 나타났다. 국내 하폐수처리장에 유입되는 질소 부하의 많은 부분을 차지하는 것은 축산폐수, 음폐수, 매립지 침출수, 산업폐수 등 기존의 하수고도처리공정으로는 때로 대응이 곤란한 악성폐수로 이에 대한 대안으로 화학적 방법에 기반한 분산형 질소 제어기술의 보급이 필요하다. 본 발표에서는 생물학적 질소제어 기술의 대안으로서 전기화학적인 방법에 기반한 암모니아성 질소 제어기술에 대한 기술개발 동향에 대해 소개한다. 하폐수 중에 존재하는 염소이온은 적절한 인가전압 하에서 자유염소로 산화되며 이들은 클로라민을 중간생성물로 하는 Breakpoint Chlorination Pathway 에 의해 질소가스와 질산성 질소로 변환된다. 이상적인 조건에서의 반응 동역학 모델 개발을 통해 pH, Cl/N 비율, 전류밀도 등 주요 운전 인자의 영향에 대해 예측이 가능하다. 전기화학적인 방법은 차아염소산을 주입하는 방법에 비해 클로라민의 농도가 낮은 상태로 유지되기 때문에 반응 선택성에 있어 많은 부분을 질소가스로 산화하는데에 유리한 것으로 나타났다. 또한 본 발표에서는 핵심 구성요소인 자유염소를 발생시키는 촉매 양극 안정성을 향상시키는 방법, 장기 운전시 발생하는 음극 표면의 스케일 형성 등 유지관리 시 고려사항 및 전기화학 기반 기술의 확대 적용을 위한 향후 연구 분야 등에 대해 논의한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR-5**
발표분야: Current Trends in Chemistry for Water Science and Technology
발표종류: 심포지엄, 발표일시: 목 15:20, 좌장: 조민

Copper-Based Hybrid Systems for Disinfection of Planktonic and Biofilm Cells

이창하

UNIST 도시환경공학부

The biocidal activity of Cu(II) is greatly enhanced by the addition of H2O2 or hydroxylamine (HA), which accelerates the production of cytotoxic Cu(I) and generates a reactive oxidant (cupryl ion, Cu(III)) capable of exerting oxidative cell damages. The bimetallic Fe-Cu nanoparticles also exhibit excellent biocidal activity in the similar biocidal mechanism. These copper-based hybrid disinfection systems were assessed for their potential to inactivate surrogate bacteria and viruses. In addition, combinations of Cu(II) with HA and H2O2 (i.e., Cu(II)/HA, Cu(II)/H2O2, and Cu(II)/HA/H2O2 systems) were tested for the control of bacterial biofilms on reverse osmosis (RO) membranes. The detailed mechanisms for the cell inactivation by different copper-based disinfection systems were discussed.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS1-1**

발표분야: [특별심포지엄]University Chemistry Education, 100 Years in Korea: "Past, Present, and Future"

발표종류: 심포지엄, 발표일시: 목 09:00, 좌장: 이원용

2050을 향한 화학인재육성

전승준

고려대학교 화학과

미정

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS1-2**

발표분야: [특별심포지엄]University Chemistry Education, 100 Years in Korea: "Past, Present, and Future"

발표종류: 심포지엄, 발표일시: 목 09:40, 좌장: 이원용

우리나라 초기의 화학교육

이대운

연세대학교 화학과

미정

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS1-3**

발표분야: [특별심포지엄]University Chemistry Education, 100 Years in Korea: "Past, Present, and Future"

발표종류: 심포지엄, 발표일시: 목 10:20, 좌장: 이원용

화학교육의 새 부대

김희준

광주과학기술원(GIST) 기초교육학부

미정

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-1**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 13:10, 좌장: 이영호

Chemistry is central to new TB diagnostics

Carolyn R. Bertozzi

Stanford University and HHMI

Tuberculosis is the world’s most lethal infectious disease and remains a global health crisis. All phases of disease management are fraught with inadequacies, including methods for point-of-care diagnosis in low resource settings that remain essentially unchanged for the past 100 years. This presentation will focus on new methods for detecting live M. tuberculosis in patient sputum samples using knowledge of mycobacterial cell wall biosynthesis and principles of physical organic chemistry.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS2-2**

발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences

발표종류: 심포지엄, 발표일시: 금 13:50, 좌장: 이영호

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

현택환

서울대학교 화학생물공학부, Center for Nanoparticle Research, IBS

Over the last 18 years, our laboratory has focused on the designed chemical synthesis, assembly and applications of uniform-sized nanocrystals. In particular, we developed a novel generalized procedure called as the “heat-up process” for the direct synthesis of uniform-sized nanocrystals of many metals, oxides, and chalcogenides.[1]

For the last 10 years, our group has been focused on medical applications of various uniform-sized nanoparticles. Using 3 nm-sized iron oxide nanoparticles, new non-toxic MRI contrast agent was realized for high resolution MRI of blood vessels down to 0.2 mm.[2] We fabricated tumor pH-sensitive magnetic nanogrenades composed of self-assembled iron oxide nanoparticles and pH-responsive ligands for theranostic application, enabling the visualization of small tumors of < 3 mm via pH-responsive T1 MRI and fluorescence imaging and superior photodynamic therapeutic efficacy in highly drug-resistant heterogeneous tumors.[3] We demonstrated that intravenously administered ceria nanoparticles could substantially reduce the damage from ischemic strokes,[4] and that triphenylphosphonium-conjugated ceria nanoparticles can localize to mitochondria and suppress neuronal death in 5XFAD transgenic Alzheimer’s disease mouse model.[5]

I will present recent advances on the fabrication of ultraflexible and stretchable electronic and optoelectronic devices integrated with various functional nanomaterials and their applications to wearable and implantable healthcare devices. We reported graphene-hybrid electrochemical devices integrated with thermo-responsive micro-needles for the sweat-based diabetes monitoring and feedback therapy.[6] We reported the designed fabrication of multifunctional wearable electronic devices for sensing, data storage, and drug-based feedback therapy of motion-related neurological disorders such as Parkinson’s disease.[7]

We introduced electromechanical cardioplasty using an epicardial mesh made of electrically conductive and mechanically elastic silver nanowire-rubber composite material to resemble the innate cardiac tissue and confer cardiac conduction system function.[8]

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2. “Large-scale Synthesis of Uniform and Extremely Small-sized Iron Oxide Nanoparticles for High-resolution T1 MRI Contrast Agents,” *J. Am. Chem. Soc.* **2011**, 133, 12624.
3. “Multifunctional Tumor pH-Sensitive Self-Assembled Nanoparticles for Bimodal Imaging and Treatment of Resistant Heterogeneous Tumors,” *J. Am. Chem. Soc.* **2014**, 136, 5647.
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대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-3**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 14:20, 좌장: 이영호

Recent Progress on Fluorescent Probes and Activable Photosensitizers

윤주영

이화여자대학교 화학·나노과학과

Fluorescence is an important detection method due to its simplicity and high detection limit.[1] Fluorescent probes have become powerful tools that allow biologists to study biological processes because they can provide visual information in real time with high spatial resolution. In this presentation, we focus our recent contributions to fluorescent chemosensors and imaging probes for ROS for various biologically important species. For example, HOCl is a biologically important reactive oxygen species (ROS).[1] Previous reports have shown that HOCl is involved in the oxidative burst of phagocytes, a process by which phagocytic cells generate highly reactive HOCl via the myeloperoxidase-H_2O_2-Cl- system to kill pathogens. Recently, we reported **R19S**,[2] **FBS**[3] and **PIS**[4] as new fluorescent probes for HOCl, which have high selectivity, sensitivity and short response time in a broad range of pH. The development of multifunctional reagents for simultaneous specific near-infrared (NIR) imaging and phototherapy of tumors is of great significance. A synergic methodology of phototherapy, photothermal therapy as well as imaging will be presented.[5] Finally, recent efforts on the developments of phosgene gas selective chemosensor,[6] will be presented.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-4**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 14:50, 좌장: 이영호

New Tools Towards the Efficient Difunctionalization of Alkenes and Alkynes

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Intermolecular processes involving the regio- and stereoselective formation of two new C-C bonds across alkynes and alkenes are in high demand as they provide an efficient access to tri- and tetra-substituted olefins as well as to highly functionalized alkyl species.[1] In this context, single step procedures involving bench stable reagents and catalysts are still scarce.[2] Here, we report different metal catalyzed three-component reactions of both alkynes and alkenes using alkyl halides and organoboronic acids.[3] These methods, which proceed via radical mechanisms using Pd and Ni catalysts, allow the preparation of the corresponding products under mild conditions in a regiocontrolled manner with excellent anti-selectivities. In addition, the stability of all reaction partners makes these reactions operationally simple and widely applicable.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-5**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 15:35, 좌장: 박소정

Direct Quantification of Various Biomarkers of Low Abundance with Force-based Atomic Force Microscopy

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 [6]. In particular, the mapping capability of AFM enabled us to see various biomarkers (DNA, mRNA, microRNA, antigen, and antibody) captured on surface [1,4,5]. In particular, fabricating a tiny spot (a few microns in diameter) of the capture probe enhanced the detection limit dramatically [2]. In this talk, examples for quantifying a translocated DNA down to single copy, miR-134 in a single neuronal cell will be presented.

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대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-6**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 16:05, 좌장: 박소정

Interfacial Assembly and Engineering of Ordered Functional Mesoporous Materials

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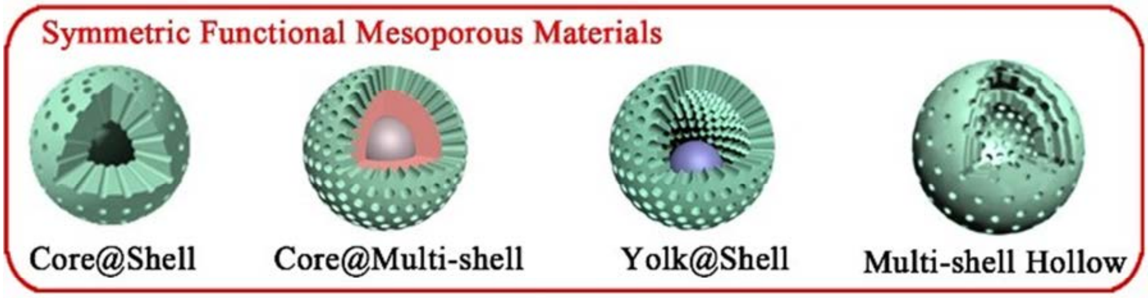
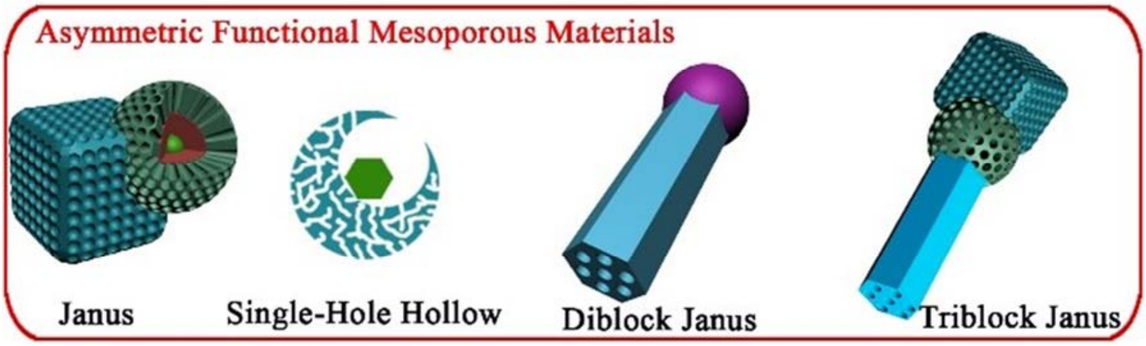
Functional mesoporous materials possess both unique properties of mesoporous materials and abundant optical, electrical, magnetic properties of inorganic nanocrystals, showing great potential in many applications. The interface plays a central role in the construction of functional mesoporous materials. Generally, two kinds of interfaces involve in the synthetic system: interface between surfactants and guest species; the interfacial interactions among solid, liquid and gas objects. Here we present the development and progress of the functional mesoporous nanomaterials by using interfacial assembly strategy. The introduction of an interfacial assembly strategy in the system can change the growth behaviors of mesoporous materials and result in the formation of novel functional mesoporous materials. Several new approaches were developed, including the liquid-liquid biphase synthesis, evaporation induced aggregation assembly, anisotropic growth strategy, *etc*. Novel mesoporous nanomaterials with multi-level architectures can be well synthesized, such as the symmetric core-shell, yolk-shell, multi-shell and asymmetric Janus, single-hole hollow, multi-blocks structures *etc*. The obtained functional materials with uniform and controllable pore channels, high surface area and open frameworks, showing great potential applications on catalysis, adsorption, separation, and biomedicine.

Figure 1. The scheme illustration of the obtained symmetric (upper) and asymmetric (bottom) functional mesoporous materials.


Symmetric Functional Mesoporous Materials


Asymmetric Functional Mesoporous Materials

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-7**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 16:35, 좌장: 박소정

Plasmon Nanogap-Engineered Nanoprobes for Photonics and Biotechnology

남좌민

서울대학교 화학부

Designing, synthesizing and controlling plasmonic nanostructures with high precision and high yield are of paramount importance in optics, nanoscience, chemistry, materials science, energy and biotechnology. In particular, synthesizing and utilizing plasmonic nanostructures with ultrastrong, controllable and quantifiable signals is key to enhanced spectroscopies, nanoantenna, plasmon-driven chemical reactions, and chemical and biological detection and biological imaging applications. Here, I will introduce newly emerging molecularly tunable and highly programmable plasmonically coupled and enhanced nanogap structures with strong, controllable and quantifiable signals including plasmonic nanogap-enhanced Raman scattering and photoluminescence. I will also show their potentials in addressing some of important challenges in science, and discuss how these new materials can lead us to new breakthroughs in biotechnologies for biosensing, bioimaging and therapeutic applications.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS2-8**
발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences
발표종류: 심포지엄, 발표일시: 금 17:15, 좌장: 박소정

Transition Metal Signaling in the Brain and Beyond

Christopher J. Chang

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Metals are essential for sustaining all forms of life, and the traditional view of this bioinorganic chemistry is that mobile fluxes of redox-inactive alkali and alkaline earth metals like sodium, potassium, and calcium are used as dynamic signals and redox-active transition metals like copper and iron are static cofactors for catalytic metabolic reactions that must buried within enzyme active sites to protect against oxidative stress. This talk will present our latest results using molecular imaging and related chemical approaches to break this narrow mold and identify novel, bonafide signaling roles for redox-active transition metals. Using copper as a primary example, we are identifying and understanding how such elements can influence neural circuitry and regulate fundamental behaviors such as eating and sleeping, as well as expanding this concept of transition metal signaling beyond neural systems.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS2-9**

발표분야: [KCS-ACS Central Science Joint Symposium] Chemistry for Next-Generation Materials and Life Sciences

발표종류: 심포지엄, 발표일시: 금 17:45, 좌장: 박소정

Can We Beat the Biotin-avidin Pair?: Ultrahigh Affinity Host-guest Complexes and Their Biological Applications

김기문

POSTECH 화학과

The high affinity and fidelity in molecular recognition and transformation is a key component of the most common biomolecules in the generation of life-like complexity and function. Apart from understanding the complexity of life, high affinity host-guest pairs have tremendous values in both biotechnology and chemical applications. The strongest and best known natural noncovalent interaction pair is the biotin–avidin (or streptavidin) system with a binding constant in the range of 10^{13}–10^{15} M^{-1}. This affinity pair has been exploited in many applications including enzyme-linked immunosorbent assays, protein and nucleic acid detection and purification, and immobilization of biomolecules on surfaces. However, it suffers some shortcomings including denaturation by organic solvents or elevated temperatures, and high cost, which prompted synthetic chemists to develop a synthetic ligand-receptor pair that can replace the biotin-avidin system in practical applications. However, the design of synthetic, monovalent host–guest molecular recognition pairs with high affinity ($K > 10^{9}$ M^{-1}) is still challenging. In this regard, cucurbit[7]uril (CB[7]), a member of the host family cucurbit[n]uril (CB[*n*], n = 5–8, 10, 14), has attracted much attention because of its ability to form ultra-stable complexes with multiple guests ($K > 10^{12}$ M^{-1}).[1] The strong hydrophobic effect between host cavity and guests, ion–dipole and dipole–dipole interactions of guests with CB portals helps in cooperative and multiple noncovalent interactions that are essential for realizing such strong complexation. These highly selective, strong yet dynamic interactions can be exploited in many applications including biomolecule immobilization, protein isolation, biological catalysis, and sensor technologies. In this talk, I will present the utility of these high affinity pairs in challenging applications especially in bio-related areas.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS3-1**
발표분야: [산학협력-동우화인켐] Wearable로 구현되는 미래화학 기술
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 최우

Future Display & Technology

김학선

UNIST

최근 인터넷 또는 영화에서 보여주는 새로운 디스플레이의 모습을 개략적으로 설명하고, 그림에서 제시하는 기법들을 소개, 미래 디스플레이를 구현하기 위한 기술들을 소개합니다. 주로 투명, 미러, Flexible, wearable, Augmant Display 등에 대한 소개와 함께 미래 기술방향에 대해 논하고자 합니다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS3-2**

발표분야: [산학협력-동우화인켐] Wearable로 구현되는 미래화학 기술

발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 최우

Optically Invisible Antennas integrated within OLED Displays using Meso-scale Conductive Polymers for Wearable Devices

홍원빈

POSTECH

Future Wearable and IoT (Internet of Things) devices with the capability of high-speed wireless communication will increasingly rely on the implementation of efficient and intelligent antennas. However, conventional wireless communication systems for small wireless electronics devices suffer from low radiation efficiencies of miniaturized antennas implemented within less-than ideal locations and real estates. This talk introduces the original concept of utilizing the entire transparent region displays to render an antenna that is completely invisible to the human eye.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS3-3**

발표분야: [산학협력-동우화인켐] Wearable로 구현되는 미래화학 기술

발표종류: 심포지엄, 발표일시: 목 14:45, 좌장: 김상태

Wearable display 현황과 중요소재기술의 이슈

조남성

한국전자통신연구원(ETRI)

1960 년대 Cathode Ray Tube, CRT 방식의 디스플레이가 국내에서 선보인 이후 플라즈마 디스플레이, 최근에 액정디스플레이까지 다양한 디스플레이들이 개발되었으며 현재 대한민국은 세계를 선도하는 디스플레이 강국으로 자리매김하고 있다. 최근 유기물을 사용하는 Organic Lighting Diode, OLED 가 차세대 디스플레이 기술로서 큰 주목을 받고 있으며 소형 및 모바일기기용 OLED 는 삼성이, 대형 OLED TV 는 LG 가 global leader 로서 그 위치를 확고히 하고 있다. OLED 관련 디스플레이 시장의 확대가 빠르게 이루어지고 있으며 다양한 응용기술들이 개발되고 있다. 여기에 디스플레이의 새로운 value 를 높이기 위한 차세대 기술로서 wearable 디스플레이에 대한 개발 요구가 크게 증가하고 있으며 다양한 소재기술부터 공정기술, 그리고 구동기술등이 필수적으로 해결되기 시작하면서 wearable 디스플레이가 점차 가시화되고 있다.

본 강연에서는 디스플레이의 개발 흐름에서 시작하여 OLED 디스플레이, 그리고 wearble 디스플레이의 개발현황을 설명하면서 필수적으로 요구되는 재료들의 개발 이슈들에 대하여 논하고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS4-1**
발표분야: [IBS 심포지엄] Genome Editing and the CRISPR/Cas Revolution (※IBS 유전체 교정 연구단 공동개최)
발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 김진수

Genome-wide target specificities of programmable nucleases in human cells

김대식 김진수*

서울대학교 화학부

Programmable clustered regularly interspaced short palindromic repeats (CRISPR) Cpf1 endonucleases are single-RNA-guided (crRNA) enzymes that recognize thymidine-rich protospacer-adjacent motif (PAM) sequences and produce cohesive double-stranded breaks (DSBs). Genome editing with CRISPR-Cpf1 endonucleases could provide an alternative to CRISPR-Cas9 endonucleases, but the determinants of targeting specificity are not well understood. Using mismatched crRNAs we found that Cpf1 could tolerate single or double mismatches in the 3′ PAM-distal region, but not in the 5′ PAM-proximal region. Genome-wide analysis of cleavage sites in vitro for eight Cpf1 nucleases using Digenome-seq revealed that there were 6 (LbCpf1) and 12 (AsCpf1) cleavage sites per crRNA in the human genome, fewer than are present for Cas9 nucleases (>90). Most Cpf1 off-target cleavage sites did not produce mutations in cells. We found mismatches in either the 3′ PAM-distal region or in the PAM sequence of 12 off-target sites that were validated in vivo. Off-target effects were completely abrogated by using preassembled, recombinant Cpf1 ribonucleoproteins.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS4-2**

발표분야: [IBS 심포지엄] Genome Editing and the CRISPR/Cas Revolution (※IBS 유전체 교정 연구단 공동 개최)

발표종류: 심포지엄, 발표일시: 수 15:20, 좌장: 김진수

Genome editing with a small Cas9 orthologue derived from Campylobacter jejuni

김은지 김진수[1,*]

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Several CRISPR-Cas9 orthologues have been used for genome editing. Here, we present the smallest Cas9 orthologue characterized thus far, derived from Campylobacter jejuni (CjCas9), for efficient genome editing in human cells and in mice. We determined protospacer-adjacent motif (PAM) sequences recognized by CjCas9 in vitro and optimized single-guide RNA (sgRNA) length in human cells. Digenome-seq, a genome-wide method for assessing off-target effects, showed that CjCas9 was highly specific, cleaving merely several sites in the human or mouse genome in vitro. Because CjCas9 is smaller than Streptococcus pyogenes Cas9 and Staphylococcus aureus Cas9, we were able to package the CjCas9 gene, its sgRNA sequence, and a marker gene in an all-in-one adeno-associated virus (AAV) vector, suggesting that CjCas9 is a promising new option for the AAV mediated gene and cell therapy.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS4-3**

발표분야: [IBS 심포지엄] Genome Editing and the CRISPR/Cas Revolution (※IBS 유전체 교정 연구단 공동 개최)

발표종류: 심포지엄, 발표일시: 수 15:40, 좌장: 김진수

In vivo genome editing with a small Cas9 orthologue derived from Campylobacter jejuni

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Here, we present Campylobacter jejuni-derived Cas9 (CjCas9) for efficient genome editing in vivo.We package the CjCas9 gene, its sgRNA sequence, and a marker gene in an all-in-one adeno-associated virus (AAV) vector and produce the resulting virus at a high titer. CjCas9, delivered via AAV, induces targeted mutations at high frequencies in mouse muscle cells or retinal pigment epithelium (RPE) cells. Furthermore, CjCas9 targeted to the Vegfa or Hif1a gene in RPE cells reduces the size of laser-induced choroidal neovascularization, suggesting that in vivo genome editing with CjCas9 is a new option for the treatment of age-related macular degeneration.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS4-4**
발표분야: [IBS 심포지엄] Genome Editing and the CRISPR/Cas Revolution (※IBS 유전체 교정 연구단 공동 개최)
발표종류: 심포지엄, 발표일시: 수 16:20, 좌장: 김진수

Highly efficient RNA-guided base editing in mouse embryos

김경미 김진수[1,*]

기초과학연구원 유전체교정연구단 [1]서울대학교 화학부

Base editors (BEs) composed of a cytidine deaminase fused to CRISPR-Cas9 convert cytidine to uridine, leading to single-base-pair substitutions in eukaryotic cells. We delivered BE mRNA or ribonucleoproteins targeting the Dmd or Tyr gene via electroporation or microinjection into mouse zygotes. F0 mice showed nonsense mutations with an efficiency of 44%-57% and allelic frequencies of up to 100%, demonstrating an efficient method to generate mice with targeted point mutations.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS4-5**
발표분야: [IBS 심포지엄] Genome Editing and the CRISPR/Cas Revolution (※IBS 유전체 교정 연구단 공동개최)
발표종류: 심포지엄, 발표일시: 수 16:40, 좌장: 김진수

Genome Editing for Plant Breeding

김상규[*] 김진수[1,*]

기초과학연구원 유전체교정연구단 [1]서울대학교 화학부

식물은 우리의 생활에 필수적인 식량자원으로 또한 의약, 공업 제품의 주요 원료로 사용된다. 식물의 생산량을 높이거나 병해충에 강한 품종을 만들기 위해 자연계에 존재하는 다양한 유전자원을 이용하여 새로운 품종을 만들고 있다. 또한, 식물 분자생물학의 발전으로 인해 외부 유전자를 식물에 도입하여 제초제 저항성, 병해충 저항성, 혹은 유용 물질을 다량으로 생산하는 식물도 만들 수 있게 되었다. 하지만 인위적으로 외부 유전자가 들어간 식물은 유전자변형(GM)식물로 분류되어 시장에 나오기까지 천문학적인 돈이 들어가는 안전성 시험 및 소비자들의 심리적 장벽을 통과해야만 한다. 이 시간에는 새로운 유전자교정기술인 크리스퍼(CRISPR/Cas) 시스템이 어떻게 기존 유전자변형식물이 가지는 한계를 극복하면서 새로운 작물을 만드는 데 사용되고 있는지 이야기하려고 한다. 특히, 식물의 물질대사 과정을 이해하고 그것을 조절하는 과정에 유전자교정기술이 어떻게 사용되고 있는지 이야기하고 앞으로의 응용 가능성을 제시하고자 한다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **KCS5-1**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 14:30, 좌장: 천철홍

Pd-Catalyzed Regioselective Synthesis of 3-Arylindoles

고태윤 윤소원*

한양대학교 화학과

Due to their various biological properties and broad applications in material sciences, indoles are one of the most important heterocycles. Especially, 3-arylindoles have been utilized for the synthesis of numerous natural products and pharmacologically important compounds. Even if various methods for the synthesis of 3-arylindole derivatives have been reported for decades, more efficient synthetic methods using readily accessible starting materials are still in great demand. Recently, our group developed a highly regioselective one-pot synthesis of 3-arylindoles from styrenes and *N*-Ts-anilines using Pd catalysis, forming new C-C and C-N bonds with high efficiency.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-2**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 14:40, 좌장: 천철홍

One-Pot Sequential Catalysis for the Synthesis of *O*-Heterocycles

유현지 윤소원*

한양대학교 화학과

Phthalides and isocoumarins are important *O*-heterocycles serving as versatile building blocks and pervasive motifs in many bioactive natural products. Therefore, a number of synthetic strategies have been developed for their construction. Also, N-heterocyclic carbenes (NHC) have been an important and influential class of organocatalysts. Previously, we reported an efficient NHC-catalyzed domino oxidation/oxa-Michael addition reaction of 2-alkenylbenzaldehydes under aerobic conditions for the easy preparation of a wide range of 3-substituted phthalides. Subsequently, we also have developed an asymmetric domino multicatalysis for the synthesis of chiral 3-substituted phthalides by using mutually compatible and cooperative catalyst system consisting of two organocatalysts, achiral NHC and chiral bifunctional cinchonine. In parallel with our efforts towards developing new synthetic methods for the preparation of various heterocycles by using NHC organocatalysts and metal catalysts, we were interested in developing a new one-pot sequential catalysis combining NHC and transition metal catalysis for the synthesis of *O*-heterocycles such as phthalides and isocoumarins. Herein we report our recent results of the investigations into this one-pot process.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-3**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 14:50, 좌장: 천철홍

Transition Metal Catalyzed Synthesis of Amides and Amines Through Alcohol Activation

이정빈 홍순혁*

서울대학교 화학부

Atom-economical amide synthesis is one of the top challenges in synthetic organic chemistry. The amide bond is the key backbone of all natural peptides in biological systems and is also an important functional group in all branches of organic chemistry. Traditionally, amides have been synthesized by reactions of carboxylic acids and their derivatives with amines, which suffers from harsh conditions and a large amount of byproducts. Over the past few years, chemists have extensively addressed new methodologies for the formation of amide bonds, aiming more efficient and environmentally benign pathway.During our studies on the atom-economical and environmentally benign amidation from alcohol with amine catalyzed by ruthenium-based organometallic complexes, we developed new amide and secondary amine bond synthetic methods from different N- or alcohol source. Amides were formed directly from azides in place of amines and we also developed a method which converts esters to amides and secondary amines in one-pot. In ester activation method, amide was formed by ester-amide exchange which generates alcohol in situ which is subsequently transformed to secondary amine via hydrogen autotransfer. These synthetic protocols with high atom economy generates hydrogen or water as the non-harmful by-products, expanding the synthetic versatility and efficiency of amide and amine bond formation.1 Z. Fu, J. Lee, S. H. Hong, Org. Lett., 2012, 14, 6028-6031.2 J. Lee, S. Muthaiah, S. H. Hong, Adv. Synth. Catal. 2014, 356, 2653-2660.3 R. Larock, Comprehensive Organic Transformations, Wiley-VCH, New York 1999.4 a) T. Ohshima, Y. Hayashi, K. Agura, Y. Fujii, A. Yoshiyama, K. Mashima, Chem. Commun. 2012, 48, 5434; b) B. Gnanaprakasam, D. Milstein, J. Am. Chem. Soc. 2011, 133, 1682-1685.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS5-4**

발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis

발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 천철홍

Selective *N*-Sulfonyl Enaminone Synthesis from Sulfonamides and Ynones by Controlling the Nature of Au(I) and Au(III) Catalysis

이다본 홍순혁*

서울대학교 화학부

N-Sulfonyl enaminones are widely utilized synthetic precursors in chemistry and biology. However, previous syntheses have significant limitations mainly on preparing starting materials and controlling selectivity among several possible isomers. Herein, we report a novel and practical method for the synthesis of *N*-sulfonyl enaminones from easily accessible substrates, sulfonamides and ynones. This method affords two different regioisomers of *N*-sulfonyl enaminones via chemoselective nucleophilic addition controlled by different catalytic systems taking advantage of the different natures of gold(III) and gold(I) catalysts. The desired regioisomers were obtained selectively by modulating catalytic systems. Moderate to excellent yields and selectivity were achieved with wide range of substrates.

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장소: 일산 KINTEX
발표코드: **KCS5-5**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 15:10, 좌장: 천철홍

Palladium(II)-Catalyzed Transformation of 3-Alkylbenzofurans to [2,3’-Bibenzofuran]-2’(3’H)-ones: Oxidative Dimerization of 3-Alkylbenzofurans

조범신 정영근[1,*]

서울대학교 화학과 [1]서울대학교 화학부

An unprecedented oxidative dimerization by palladium catalysis has been developed using PhI(OPiv)2 as a by-standing oxidant. This provides a facile method for the synthesis of quaternary 2,3’-bibenzofuran-2’(3’)-ones from readily acces-sible substrates. A plausible mechanism involving a Pd(II)-Pd(IV) catalytic cycle is proposed; a trace amount of water is required for subsequent oxidation.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **KCS5-6**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 15:20, 좌장: 천철홍

Cobalt-rhodium heterobimetallic nanoparticle-catalyzed reactions

정현호

서울대학교 자연과학대학 화학부

Transition metal nanoparticles have attracted a great leal of attention. Co-Rh nanoparticles (Co_2Rh_2) with a fixed stoichiometry (2:2) were easily obtained from $Co_2Rh_2(CO)_{12}$. At first, The nanoparticles were quite effective catalysts for carbonylation reaction. Particularly, special focus was paid to the Pauson-Khand reaction. But now, the nanoparticles are also quite effective catalysts for hydrogenation and dehydrogenation.

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발표코드: **KCS5-7**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 15:30, 좌장: 천철홍

Synthesis of symmetric and asymmetric multi naphthol dendrimeric compounds

김재웅 오창호*

한양대학교 화학과

Jaewoong Kim and Chang Ho Oh*Department of Chemistry, Hanyang University, Wangsimni-ro 222, Seongdonggu, Seoul 04763, KoreaAu-catalyzed cyclization of two propargylic carboxylate was developed by our lab. Au-activated di alkynyl phenyl compound b was transformed to naphthyl compound c. To extend this c for multi naphthyl compounds, naphthol compounds d (deprotected acetyl group) was applied for dendron, reacted with TCT(cyanuric chloride) and multi bromo alkyl compounds. In short, multi naphthyl compounds, having conjugated and non-conjugated central system, were synthesized. Finally, multi hydroxyl dendrimeric compounds were synthesized via MOM deprotection.

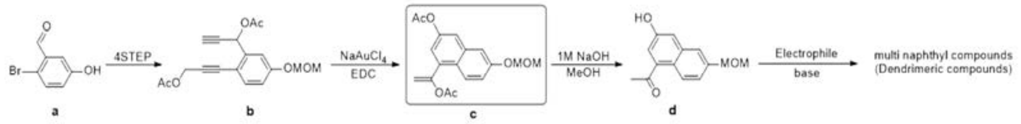


fig 1. Overall scheme of O-protected multi naphthyl substrates

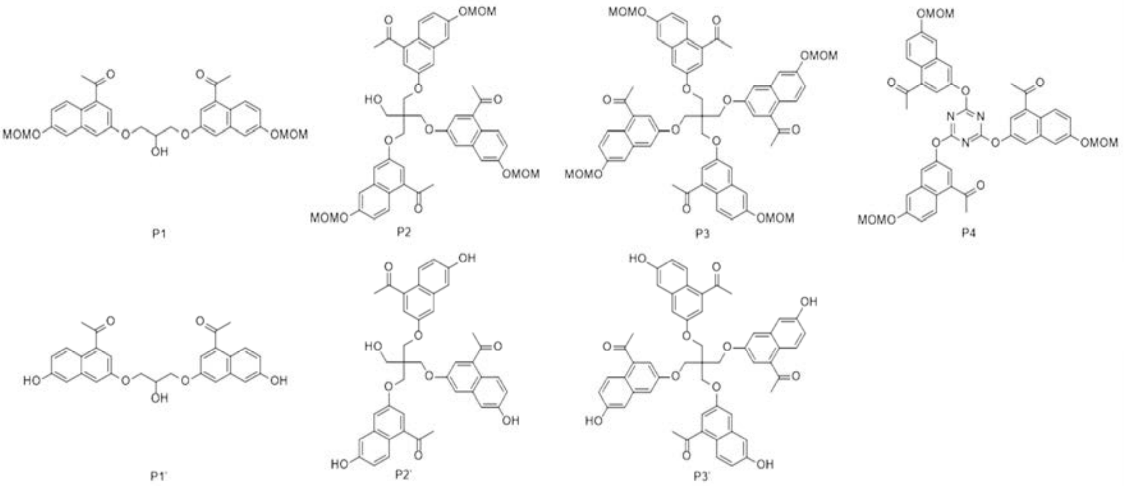


fig 2. 4 Types of dendrimeric compounds

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS5-8**

발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis

발표종류: 심포지엄, 발표일시: 수 15:40, 좌장: 천철홍

Visible-Light-Induced [4 +2] benzannulation

이다슬 조은진*

중앙대학교 화학과

Polycyclic aromatic and heteroaromatic compound have received tremendous attention due to their various biological, electronic properties and have been utilized as the important structural motifs in many applications. In particular, because of their strong fluorescence emission property, they have been applied to various electronic devices such as OLEDs, OFETs. We have synthesized a library of polycyclic aromatic and heteroaromatic compound through visible-light induced [4+2] benzannulations between 2-(hetero)aryl-substituted anilines and (hetero)aryl alkynes in the presence of fac-Ir(ppy)3 as the photocatalyst and tBuONO as the diazotization reagent. The in situ generation of diazonium salt as intermediate allowed extended substrate scope that have not been easy to access. In this talk, the detailed study on chemo- and regio-selective [4+2]-benzannulation to synthesize highly substituted tricyclic- and tetracyclic compounds including phenanthrene derivatives will be presented.

- ➢ **synthesis of library of polycyclic (hetero)aromatics**
- ➢ **chemo- and regioselective synthesis**
- ➢ **broad substrate scope with high functional group tolerance**
- ➢ **gram-scale synthesis**

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

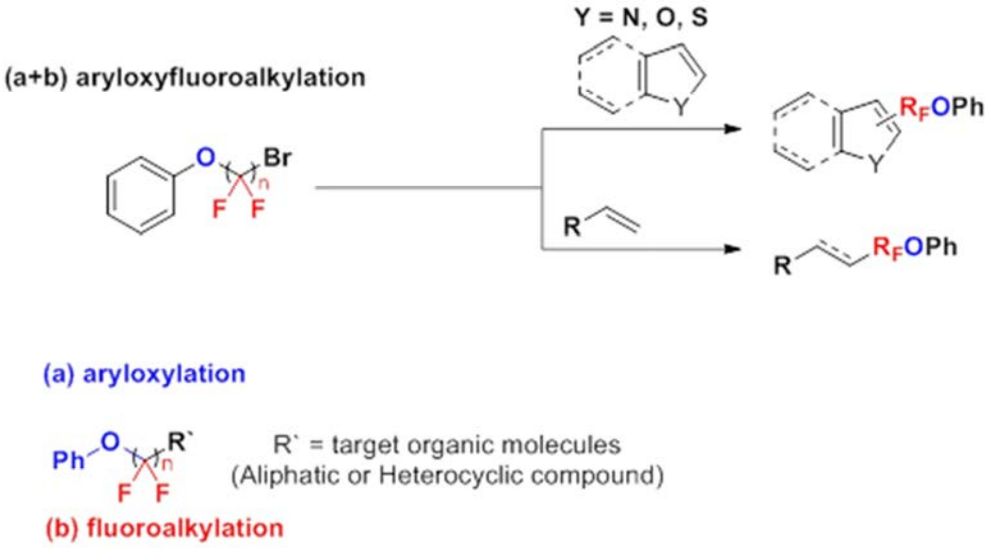
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-9**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 15:50, 좌장: 천철홍

Visible-Light-Induced Aryloxyfluoroalkylations

박귀림 조은진*

중앙대학교 화학과

Installation of fluoroalkyl groups has been of great interest in many fields because of their ability to change the physical, chemical, and biological properties such as lipophilicity, binding selectivity, metabolic stability and bioavailability. In particular, the introduction of fluoroalkyl groups containing oxygen has been of growing interest because the presence of oxygen can further change the properties of molecules. We have developed a visible light-induced oxyfluoroalkylations under mild reaction conditions. By this approach, two functional groups consisting of oxygen and fluoaoalkyl moieties could be simultaneously installed to various organic molecules, showing the potential use of the method for late-stage modifications in the development of functional molecules. In addition, this method can be easily utilized for fine-tuning of properties in drug development by controlling the number of fluorine atoms in reagents



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

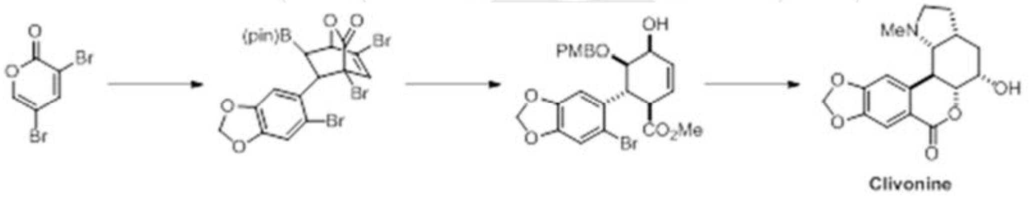
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-10**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 16:20, 좌장: 홍순혁

Recent 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, we have further envisioned that the aforemen-tioned synthetic strategy should be also effective for clivonine. Our efforts toward this natural product will be discussed.



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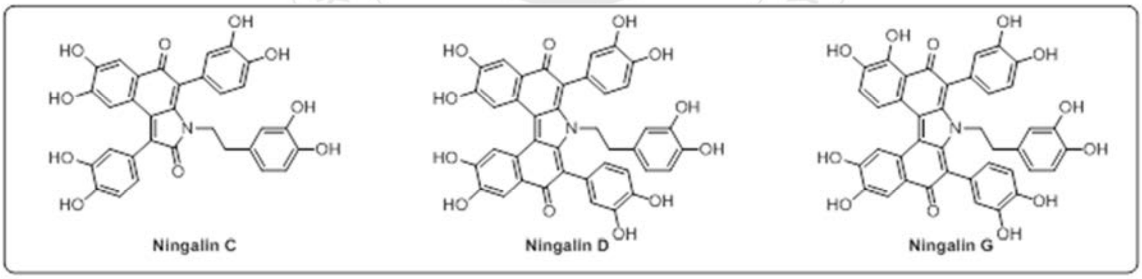
장소: 일산 KINTEX
발표코드: **KCS5-11**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 16:30, 좌장: 홍순혁

Total synthesis of Ningalin C, D and G

<u>김장엽</u> 조천규*

한양대학교 화학과

In conjunction to our ongoing study on aryl hydrazides, we have elaborated a new synthetic route to marine alkaloid ningalin C, D and G by way of dibenzo-carbazoles that are readily accessible from dinaphthyl hydrazides via [3,3]-sigmatropic rearrangement followed by cyclization of the resulting diamine products. Introduction of 3,4-dimethoxyphenyl groups and oxidations would complete the total syntheses of the above marine alkaloids. Presented herein will be our recent efforts toward the synthesis of poly-substituted naphthalenes and application to the synthesis of ningalin C, D and G



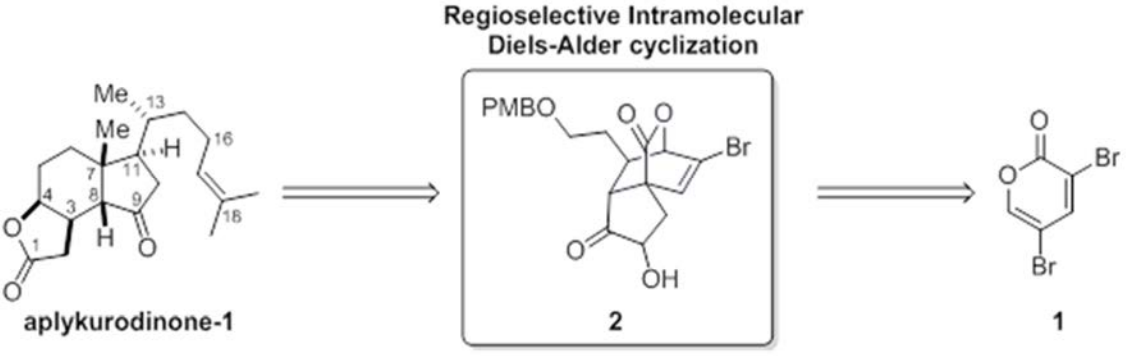
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-12**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 16:40, 좌장: 홍순혁

Total synthesis of aplykurodinone-1 by Efficient Regio-selective Intramolecular Diels-Alder of 2-pyrone

이준호 조천규[1,*]

한양대학교 자연과학 화학과 [1]한양대학교 화학과

Aplykurodines are steroids natural products which have tricyclic ring core. Many aplykurodines show cytotoxic activities against a range of human cancer cell lines . Natural product aplykurodinone-1 which we eager to synthesize have a unsaturated side chain linked to the unusual cis-fused hydrindane moiety with six contiguous stereocenters.As a part of our ongoing study on 3,5-dibromo-2-pyrone toward target oriented synthesis, we devised a new synthetic route to aplykurodinone-1 by way of tricyclic lactone that we envisioned to access with an intramolecular Diels-Alder reaction of 2-pyrone containing vinyl ketone group as dienophile. The IMDA reaction indeed allowed us to the key tricyclic lactone intermediate. Subsequent reactions including lactone ring opening will culminate in the total synthesis of the titled natural product.



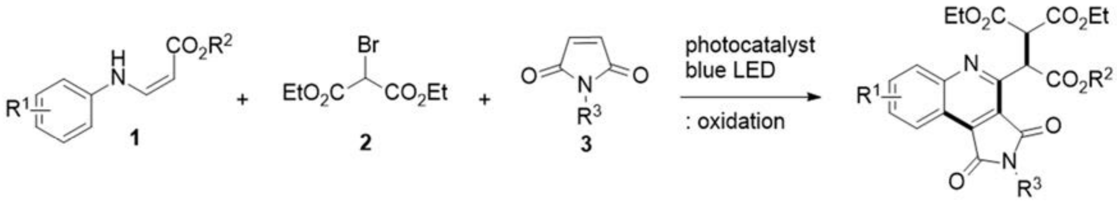
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-13**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 16:50, 좌장: 홍순혁

Three-Component Synthesis of Quinolines based on Visible-Light Photoredox Catalysis

최준호 박철민*

UNIST 화학과

Recently, irradiation of visible light photoredox catalyst has been widely used to drive transformation of organic molecules though the highly desirable processes. Photocatalysts absorb visible light to provide stable, long-lived photo-excited states. The conversion of these excited states to the bench states induces single-electron-transfer events providing access to radical ion intermediates having reactivity patterns fundamentally different from those of their ground electronic or excited states. Multicomponent reactions (MCR) serve as a powerful tool, employing three or more simple building blocks to produce complex molecular frameworks in a single step. Photoredox catalysis has been explored in the context of MCR. However, the limited examples are mostly based on radical-polar crossover mechanisms, in which the process is in operation for initial coupling of two reactants, while a third component is incorporated via a polar process. Although this approach is useful, quenching of radical processes by redox catalysts entailing the involvement of polar processes poses limitations in the scope of coupling partners. To the best of our knowledge, MCR with three consecutive bond formation based on radical processes via visible-light photoredox catalysis has not been reported.Due to their utilities, significant efforts have been made to develop efficient synthetic methods for quinolines. However, the conventional methods rely on condensation under harsh conditions and more recent developments are limited to transitional metal-catalyzed and iodine-mediated synthesis. Here, a successful development of a new tandem radical cyclization based on visible-light photoredox catalysis enables the efficient formation of quinolines based on consecutive radical processes.



R¹
H
N
CO₂R²
1
+
Br
EtO₂C
CO₂Et
2
+
O
N
O
R³
3
photocatalyst
blue LED
: oxidation
EtO₂C
CO₂Et
N
CO₂R²
R¹
O
N
O
R³

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-14**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 17:00, 좌장: 홍순혁

Development of Novel Synthetic Routes for Axially Chiral BISESAMOL 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 chiral building blocks in chiral Brønsted acid catalysis. 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 the diastereomeric resolution of BISESAMOL boronic acid using a boronic acid moiety as a resolving group. Subsequent derivatization of the boronic acid moieties 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, 81, 8464.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-15**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 17:10, 좌장: 홍순혁

A Novel Synthetic Route for Indoloquinolizine Derivatives via Cyanide-Catalyzed Imino-Stetter Reaction

박은준 천철홍*

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. One of the most common methods to access the core indoloquinolizine structure is the Pictet-Spengler reaction of imines derived from tryptamine and aldehydes. Another one is the Bischler-Napieralski reaction of 3-piperidioneindole derived from tryptamine and furancarboxylic acid. However, these methods generally require additional steps to generate another six-membered ring and toxic metals for coupling reactions.Recently, our group developed a new method for the synthesis of 2-substituted indole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and aldehydes via cyanide-catalyzed intramolecular imino-Stetter reaction. 1,2 We further extended this protocol to the synthesis of indole-3-acetic acid derivatives bearing a pyridyl moiety at the 2-position from aldimines obtained from 2-aminocinnnamic acid derivatives and various pyridinecarbaldehydes. Subsequent reduction of the carboxylic acid moiety to an alcohol followed by cyclization to provide tetrahydro-indoloquinolizines. Following reduction of the pyridinium ring with several nucleophiles afforded the expected indoloquinolizines. In this presentation, we will describe our new approach towards the preparation of indoloquinolizine scaffold. Reference1. Lee, S. J.; Seo, H.-A.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 1566.2. Seo, H.-A.; Cheon, C.-H. J. Org. Chem. 2016, 81, 7917.

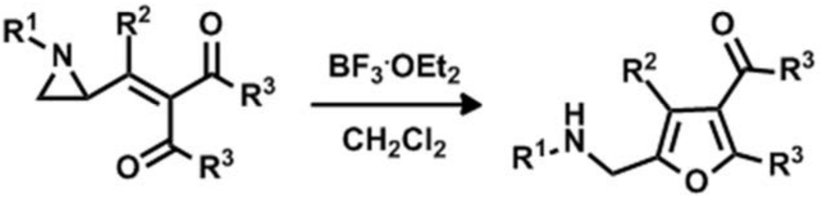
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-16**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 17:20, 좌장: 홍순혁

Transition metal free synthesis of polysubstituted aminomethylfuran from aziridines

정현수 Nagendra Nath Yadav[1] 하현준[2,*]

한국 외국어 대학교 화학과 [1]North Eastern Regional Institute of Science And Technology, Department of Chemistry [2]한국외국어대학교 화학과

Transition metal free and highly atom economical synthesis of polysubstituted furan were achieved via aziridine ring-opening in good to excellent yields. The resultant aminomethylfuran derivative was used for one-pot Micheal reaction followed by Diels Alder reaction to get complex polycyclic heterocycles in good yields.



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

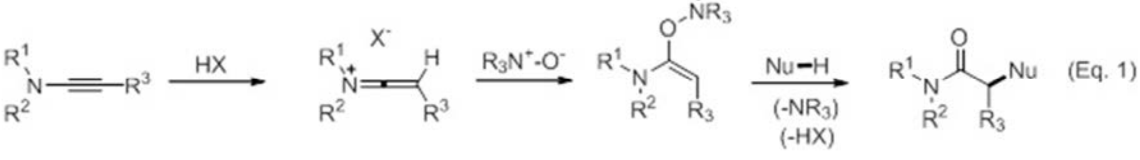
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS5-17**
발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis
발표종류: 심포지엄, 발표일시: 수 17:30, 좌장: 홍순혁

An Organocatalytic Approach toward Carbene Synthons

PATILDILIPVITTHAL 신승훈*

한양대학교 화학과

Alkyne oxidation chemistry, pioneered in Au and Rh catalysis, has enables access to α-oxo carbene synthons and thereby mediates a variety of C-X bond formations, C-H functionalizations and cyclopropanations. In this presentation, we report a simple and robust strategy to access α-oxo carbene equilvalent under Brönsted acid catalysis. Inspired with pioneering work on acid-catalyzed generation of keteniminium ions by Hsung and Kozmin as well as transition metal-catalyzed α-oxo carbene chemistry, we envisioned Brønsted acid catalyzed ‘enolate umpolung’ strategy for intermolecular coupling of ynamide with different nucleophiles, that would result in α,α-di(hetero)aryl amide which are one of the most widely occurring structural motifs in various biologically active compounds, natural products, and electro-optical materials. It is intriguing because such non-metal approach has been limited only to intramolecular cases so far, because an intermolecular version requires chemoselective differentiation of possible nucleophilic species.We found that easily available ynamides can serve as an excellent substrates in the presence of catalytic amount of Brönsted acid giving keteniminium ions, followed by N-oxide attack and intermolecular Friedel Craft addition to the umpolung enolate, with remarkable ease (RT, 1~2 h) (Eq. 1). This simple yet robust synthetic methodology is applicable to wide range of nucleophiles such as indoles, pyrroles, phenols and silyl-enol ethers in good to excellent yields (45-98 %).



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS5-18**

발표분야: [SRC 심포지엄] New Trends and Developments in Organic Synthesis

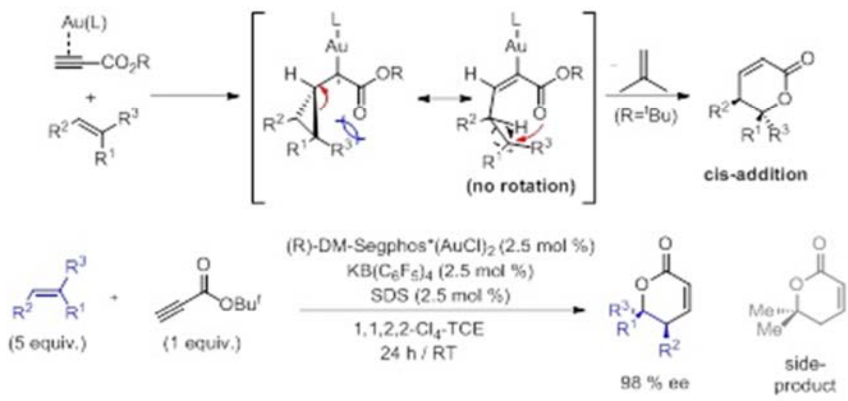
발표종류: 심포지엄, 발표일시: 수 17:40, 좌장: 홍순혁

Remarkable Effect of Solvent and Surfactant in Intermolecular Gold-Catalyzed Enantioselective [4+2] Cycloaddition

김한별 신승훈*

한양대학교 화학과

α,β-Unsaturated-δ-lactones are found in a number of biologically active natural products, such as fostriecin, leustroducsin, and pironetin. Traditional methods for the synthesis of the key scaffold involve hetero Diels-Alder and ring-closing metathesis among others. In our previous work, it was found that propiolic acids function as an equivalent of a 1,4-C,O-dipole for [4+2] annulation of α,β-unsaturated-δ-lactones. Here a mediocre enantioselectivity (upto 65 %ee obtained with DM-Segphos) indicates a challenge in asymmetric Au(I)-catalyzed intermolecular reaction. Enantio-discriminating step in this reaction presumably involves prochiral facial discrimination of the olefin nucleophile which is positioned away from the chiral ligand on gold. Our initial efforts to modify the chiral backbone of the ligand resulted on only poor enantioselectivity. However, change of solvent and counter-anion had profound effect on the enantioselectivity and we identified 1,1,2,2-tetrachloroethane and KB(C6F5)4 as the optimal combination of solvent and counter-anion. Although 80~98%ee was achieved under these conditions, some substrates still gave poor yields (20~50 %), presumably because of the side product resulting from the liberated isobutene. After extensive experiments, we found that addition of surfactants had beneficial effects on yields with some substrates giving higher enantioselectivity as well. Updates on the effect of amphiphile in terms of olefin substrate classes as well as the possible explanation for this effect will be discussed in this presentation.


Au(L)
CO₂R
+
R²
R³
R¹
L
Au
H
OR
O
R²
R¹
R³
L
Au
H
OR
O
R²
H
R¹
R³
(no rotation)
(R=ᵗBu)
O
O
R²
R¹
R³
cis-addition
R³
R²
R¹
(5 equiv.)
+
O
OBuᵗ
(1 equiv.)
(R)-DM-Segphos*(AuCl)₂ (2.5 mol %)
KB(C₆F₅)₄ (2.5 mol %)
SDS (2.5 mol %)
1,1,2,2-Cl₄-TCE
24 h / RT
O
O
R³
R¹
R²
98 % ee
O
O
Me
Me
side-
product

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS6-1**
발표분야: [튜토리얼] Practical Course of Structure Analysis by Single Crystal X-ray Diffraction
발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 이윤호

Practical Course of Structure Analysis by Single Crystal X-ray Diffraction

박기민

경상대학교 기초과학연구소

단결정의 X-선 회절 데이터에 기초한 구조해석은 명확한 분자의 구조 뿐만 아니라 초분자 상호작용을 알 수 있다는 점 때문에 초분자화학의 전성기와 맞물려 많은 연구자들이 선호하는 연구 수단중의 하나가 되었으며, 이런 이유로 국내에도 많은 단결정 X-선 회절장치가 보급되어 있다. 하지만 단결정 X-선 회절장치를 이용해 얻은 회절 데이터의 처리 및 해석을 통해 자신의 연구에 필요한 정확한 정보를 얻어내는 것에 있어서는 많은 연구자들이 어려움을 겪고 있는 실정이다. 이는 단결정 X-선 구조해석을 위한 체계적인 교육 프로그램이나 강의가 없기 때문이다. 이런 문제점을 조금이나마 해소해 보고자 X-선 단결정 구조해석 실무교육을 실시한다, 이번 교육과정에서는 측정데이터 (raw data)로부터 구조해석 파일들(ins, hkl, lst, res)의 형성과정과 파일 내의 내용들이 가지는 의미, 구조해석의 진행과정 그리고 최종 구조해석의 완성을 담은 cif 파일의 작성까지 실제 데이터를 이용하여 구조해석의 시작에서 마무리까지 초보자들도 알기 쉬운 내용으로 진행할 예정이다. 또한 시간적인 여유가 있다면 초분자 상호작용을 이해하기 위한 소프트웨어(Mercury, PLATON)의 활용법에 대해서도 간단히 다룰 것이다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS7-1**
발표분야: 대학원생들을 위한 실험실 안전교육
발표종류: 심포지엄, 발표일시: 목 13:30, 좌장: 이익모

연구실 사이버 보안

이소영

교육부 정보보호팀

사회전반의 정보통신 기술에 대한 높은 의존도로 사이버 침해사고가 우리 사회 전반에 직·간접적인 위해를 가하고 있다. 이에 따라 개인정보 유·노출 사고에 따른 침해, 연구 결과자료, 기밀정보 등 중요자료 유출 및 탈취, 사이버 침해 사고로 인한 시스템 마비 등 사이버 공간의 위험은 다양하게 증가하고, 그에 따른 가정과 사회생활에서의 해당 분야별 혼란과 피해 범위도 넓어지고 있다.

이에 따라 교육기관의 사이버 침해 위협도 지속적으로 증가되고 있는 상황으로 '교육부 사이버안전센터'에서 관제한 사이버 침해 위협 탐지 건수는 전년도 대비 7% 정도 증가추세에 있다. 교육기관의 사이버 침해 사고에는 대학 연구실에서의 연구 활동에 활용되는 서버, 노트북, 연구성과물 등 연구자원의 피해 사례도 상당수 포함되어 있다. 따라서 이러한 침해 사고 유형 및 사고 예방책에 대하여 논의하고자 한다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS7-2**
발표분야: 대학원생들을 위한 실험실 안전교육
발표종류: 심포지엄, 발표일시: 목 14:10, 좌장: 이익모

Protection of researchers from the risks of carcinogen exposures in labs

박정임

순천향대학교 환경보건학과

This presentation will discuss about when laboratory researchers are or likely to be exposed to carcinogens. Researchers who work in chemistry R&D laboratories use various chemicals including carcinogens and epidemiological studies have reported the association between laboratory workers and excessive cancer mortalities. The nature, degree and duration of exposure to hazardous chemicals among laboratory workers should be determined in order to assess any risks and to protect laboratory workers' health. Exposure assessment and characterization for laboratory workers, however, has not been properly addressed partly because the laboratory working conditions are unlike typical industrial settings, i.e., frequently changing tasks, multiple chemicals in use simultaneously, irregular work schedules, etc. Upon recognizing the significance of exposure assessment, Laboratory Safety Act in Korea has recently added legal requirements of performing exposure assessment of hazardous chemicals. A couple of topical studies will be introduced in this presentation: 1) case studies conducted in order to investigate how many and what kind of carcinogens are in use, 2) exposure characterization of volatile organic compounds (VOCs) in chemistry research laboratories.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS7-3**

발표분야: 대학원생들을 위한 실험실 안전교육

발표종류: 심포지엄, 발표일시: 목 14:50, 좌장: 이익모

유기화학 실험실 안전관리 매뉴얼

김현진

한국화학연구원 의약바이오연구본부 친환경신물질연구센터

한국화학연구원 의약바이오연구본부에서 준비한 안전관리 교육으로서 유기화학 실험실에서 발생 가능한 사고사례에 대한 분석 및 예방 방법에 대한 교육을 골자로 합니다. 본 발표는 연구를 시작하는 대학원생 및 연구원들을 대상으로 하며, 주제는 실험 수행 전 지켜야 할 안전 수칙들과 실제 사고 사례 분석을 통한 사고 원인 교육 및 대책입니다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS8-1**

발표분야: ACS Special Session

발표종류: 심포지엄, 발표일시: 수 15:00, 좌장: 미정

[발표취소] 미정

Qiong Yuan

Business Development-Asia, CAS, a division of the American Chemical Society

발 표 취 소

본 논문은 발표취소된 논문입니다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.O-1**

발표분야: Oral Presentation for Young Polymer Scientists

발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 윤명한

Coupling Phase Separation and Gelation of Covalent Network/Polymer Mixture Toward Facile Synthesis of Nanoporous Covalent Frameworks

오왕석 배재성[1] 박지웅*

GIST 신소재공학부 [1]University of California, San Diego, U.S.A.

Coupling two different structure-forming mechanisms has been a promising strategy to generate distinctively nanostructured polymeric materials. Recently, we have reported various nanoporous polymers prepared from the polymer/Urea Network(UN) mixtures via organic sol-gel method. Monolithic and co-continuous nanoporous structures could be obtained by spinodal decomposition between polymer and UN followed by polymer extraction. To further understand the relationship between polymer and nanostructure development, we investigated the phase behaviors of polymer/UN mixtures and the resulting porous morphology with various polymers. Physicochemical properties of the polymers, compositions in the blend, and especially kinetic matching of phase separation and gelation dynamics were critical in the morphology evolution. Empirical physical parameters were employed to estimate the governing interactions and give guidance on the polymer candidates. These findings are expected to provide general criteria of polymer that leads to optimized nanoscale architecture required for specific applications.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.O-2**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 윤명한

Enhanced precision of in-vivo stable non-covalent polymergatekeepers in mesoporous silica nanoparticles for hydrophobic drug delivery in tumor therapy

<u>LOGANATHANPALANIKUMAR</u> **유자형**[1,*]

UNIST Environmental Scienc [1]*UNIST 자연과학부 화학과*

Targeted delivery mediated by ligand modified nanocarriers have been extensively pursued for cancer chemotherapy, however the efficiency is still limited by premature drug release after the administration. Herein, we represented a simple, one-pot synthesis and robust method by installing non-covalent polymer gatekeepers in mesoporous silica nanoparticles. The unmodified mesoporous silica nanocontainers have a high loading capacity for hydrophobic drugs. This is a tumor adaptable drug carrier made of disulfide bonded polyethylene glycol-pyridyl disulfide (PEG-PDS) polymer gatekeepers and can release drug upon the increased intracellular glutathione concentration. In-situ covalently crosslinked the PEG-PDS capped mesoporous silica nanoparticles have shown improved encapsulation to avoid the premature drug release. Intravenously injected non-covalent polymergatekeepers have led to hydrophobic doxorubicin in cancer cells and suppresses the tumor growth in mice. As compared to the self-assembled micelles, doxorubicin loaded polymergatekeeper mesoporous nanoparticles have shown improved tumor reducing capability.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.O-3**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 윤명한

Design of nitric oxide-responsive hydrogel

박정홍 김원종*

POSTECH 화학과

Nitric oxide (NO) is an crucial signaling molecule that regulates physiolgical conditions such as apoptosis, neurotransmission and cell vasodilation. Recently, radical ability of NO has drawn attention in various fields, including NO sensing, NO scvanger and so on. We evaluated some materials that change their physical properties by responding to NO specifically would play significant roles as NO-responsive biomaterials as well as scavengers that capture and remove NO. Therefore, we designed a novel NO-responsive hydrogel crosslinked by acryamide and nitric oxide-cleavable crosslinker (NOCCL). The hydrogel was swelled dramtically in response to NO by consuming NO. As a control, BIS hydrogel crosslinked by N,N'-methylenebisacrylamide (BIS) showed no change at even high concentration of NO. In addtion, the hydrogel was studied about its mechanical properties (G',G'') from theology test to understand responsiveness to NO. Therefore, the NO-responsive hydrogel is a new class of biomateiral that may prove to use in many applications, such as a gas detection device, a drug delivery vehicle, a modulator of inflammation and a scaffold for tissue engineering

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장소: 일산 KINTEX
발표코드: **POLY.O-4**
발표분야: Oral Presentation for Young Polymer Scientists
발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 윤명한

Fabrication of fibrillary hydrogel via partial crystallization and its application for three-dimensional neuronal network construction

김동윤 윤명한*

GIST 신소재공학부

Dissolution of polymer at solvent/polymer interface is of interest not only for fundamental science but also in the field of industry. Depending on solvent condition, the solvent/polymer interface is reached into three different equilibrium states: first, complete dissolution of the polymer in which the individual polymers are dislocated by the solvent. Second, not dissolved polymer, having an abrupt interface with respect to the solvent. Third, gel state in which the polymer is swelled with solvent. Herein, by using solvent/dissolvent (water/ethanol) mixture and electrospun poly(vinyl alcohol) (PVA), dynamic polymer dissolution process at the polymer interface is controlled and enable to modulate polymer crystallization degree. The polymer density and microstructure of hydrogel, which is measured by optical tomography and atomic force microscopy, respectively, reveal partially crystallized hydrogel structure. The resultant PVA fiber hydrogel exhibit preserved original fiber structure and decent optical transparency. Finally, the fibrillary hydrogel is used as a scaffold for artificial three-dimensional neuronal network construction.

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장소: 일산 KINTEX

발표코드: **POLY.O-5**

발표분야: Oral Presentation for Young Polymer Scientists

발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 윤명한

Photothermoelectric Properties of Thiophene-based Conducting Polymers

김병관 한민수 임한휘 김은경*

연세대학교 화공생명공학과

Conducting polymers (CPs) have been good candidate for various applications such as energy harvesting, optical imaging, and sensing devices, due to their controllable optoelectronic properties and simple processability. In particular, thin films of CPs have been shown interesting thermoelectric conversion and photothermal heat generation. The highly conductive thiophene-based π-conjugated polymers were explored to demonstrate as an photothermal materials in near-IR (NIR) range, which were used for harvesting of solar energy, harvesting of live cell sheets, and ablation of cancer cells. Due to the high photothermal effect, photo thermoelectric energy was harvested from the thin films of CPs upon exposure to NIR. The effect of polymer structure and ordering on the NIR photothermoeelctric conversion will be discussed.

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장소: 일산 KINTEX

발표코드: **POLY.O-6**

발표분야: Oral Presentation for Young Polymer Scientists

발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 윤명한

Low-Crystallinity Conducting Polymers Showing High Field-Effect Mobility

손성윤 박태호*

POSTECH 화학공학과

Conducting polymers form complicated microstructures combining crystalline and amorphous regions because of their semicrystalline nature. Crystalline regions of conducting polymers have a more regular arrangement than amorphous regions. Hence, they typically also have higher rates of charge carrier transport due to enhanced charge carrier delocalization. Thus, various studies have attempted to increase crystallinity of conducting polymers to enhance charge carrier transport. However, these approaches are inevitably limited by the semicrystalline nature of conducting polymers. Furthermore, increase in crystallinity can lead to significant decrease in mechanical resilience because cracks tend to occur at grain boundaries of crystalline domains. In this study, in an effort to improve charge carrier transport in low-crystallinity conducting polymers, we form localized aggregates in amorphous regions of the polymers by introducing thiophene monomers without alkyl chains into the polymer backbone. As a result, the resulting increase in connectivity between polymer backbones within the amorphous regions and backbone planarity give rise to enhanced inter- and intra-chain charge transport.

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장소: 일산 KINTEX

발표코드: **INOR.O-1**

발표분야: Oral Presentation of Young Inorganic Chemists

발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 이진석

Direct observation of the formation, structures, and dynamics of individual nanoparticles in solution

박정원

서울대학교 화학 생물 공학부

Nanocyrstals are widely studied for their physical properties and utilized in biology, electronics, optics, and catalyst. However, most of nanocrystal synthesis and their uses are developed empirically with a limited mechanistic understanding. It is mainly because of their size and heterogeneity in structures and physical properties which cannot be easily accessible by conventional analytical methods. Here, we introduce in situ observations of the phase transition, growth, 3D structures, and dynamics of individual nanocrystals. Our study unveils heterogeneity of growth mechanism of individual nanocrystals, critical steps during growth that incorporate non-classical pathways, and resulting 3D structures at the atomic resolution. Following their motions and interactions in solution, formation mechanism of the 2D superlattice of nanocrystals is also elucidated in a single particle resolution. Direct observation of nanocrystal motions when conjugated with biological systems is also presented along with an introduction of the methodological development that enables aforementioned studies.

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장소: 일산 KINTEX
발표코드: **INOR.O-2**
발표분야: Oral Presentation of Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 목 09:25, 좌장: 이진석

Origin and hysteresis of lithium compositional spatiodynamics within battery primary particles revealed via operando x-ray microscopy

임종우

서울대학교 화학부

The kinetics and uniformity of ion insertion reactions at the solid-liquid interface govern the rate capability and lifetime, respectively, of electrochemical devices such as Li-ion batteries. Using an operando x-ray microscopy platform that maps the dynamics of the Li composition and insertion rate in LixFePO4, we found that nanoscale spatial variations in rate and in composition control the lithiation pathway at the subparticle length scale. Specifically, spatial variations in the insertion rate constant lead to the formation of nonuniform domains, and the composition dependence of the rate constant amplifies nonuniformities during delithiation but suppresses them during lithiation, and moreover stabilizes the solid solution during lithiation. This coupling of lithium composition and surface reaction rates controls the kinetics and uniformity during electrochemical ion insertion.

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장소: 일산 KINTEX
발표코드: **INOR.O-3**
발표분야: Oral Presentation of Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 이진석

Nanotechnology meets Biology; A Mechanogenetic Toolkit for Interrogating Cell Signaling in Space and Time

서대하

DGIST 신물질과학전공

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

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **INOR.O-4**
발표분야: Oral Presentation of Young Inorganic Chemists
발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 이진석

Smoothing the Transition from Iron-Oxygen Chemistry to Iron-Nitrogen Chemistry

홍승우 남원우[1,*]

숙명여자대학교 화학과 [1]이화여자대학교 화학과

Multiply bonded terminal oxo(O^{2-}) and imido(NR^{2-}) species of transition metals have been postulated as key intermediates in many enzymatic and synthetic oxidative transformations such as olefin epoxidation and aziridination and unreactive C-H bonds oxygenation and amination.For instance, high-valent iron-oxo species have been frequently invoked in the catalytic cycle of cytochrome P450 whereas high-valent iron-imido species have been considered as a potential intermediacy in Haber-Bosch process for dinitrogen reduction process. In both enzymatic and biomimetic studies, a number of high-valent iron-oxo species accommodating heme and nonheme systems have been isolated and spectroscopically investigated; however, their congeners, high-valent iron-imido species remained relatively scarce. Moreover, the fundamental challenge lies in inferring how high-valent iron-imido species incorporate nitrogen functionality into C-H bonds including kinet-ic and mechanistic studies. To date, transition metal imido complexes such as titanium, manganese, iron, cobalt and nickel have been characterized but few are capable of activating C–H bonds and/or transferring their nitrene (-NR) group, in part, due to their low-spin nature and ligand-field stabilization energies. Motivated by scrutinizing multiply bonded terminal imido species of iron, we herein report for the first time the synthesis and spectroscopic charaterization of a high-valent iron(V)-imido complex, supported by tetraamido macrocyclic ligand.

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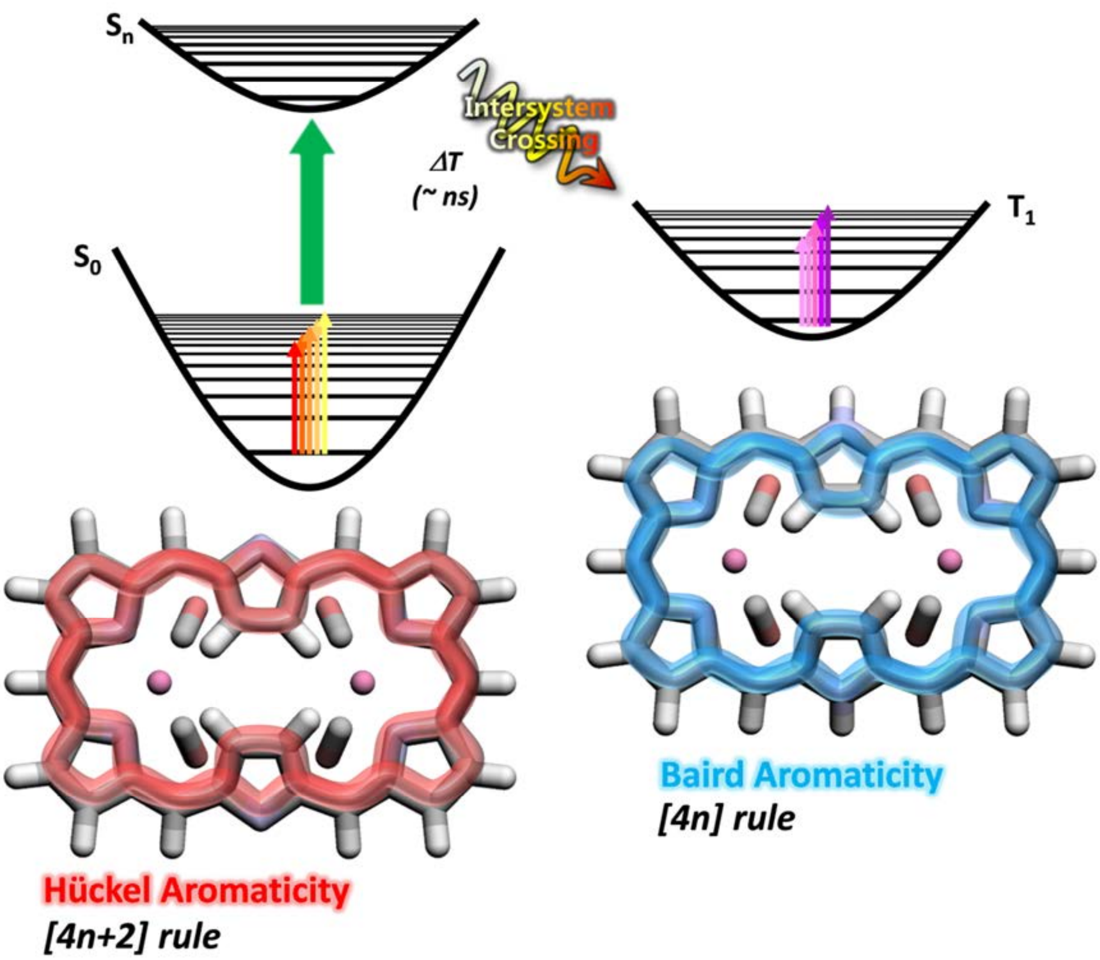
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 조성

The description of vibrational modes in hexaphyrins providing for the comprehension of aromaticity reversal in the lowest triplet state

성영모 김동호*

연세대학교 화학과

Aromaticity reversal in the lowest triplet state, or Baird’s rule, one of the most interesting concepts in the field of physical organic chemistry, has been postulated for the past few decades with the aid of theory and quantum calculations. Despite of numerous theoretical works on aromaticity reversal, experimental study for aromaticity reversal is still in the rudimentary stage. Thus, here, we have investigated the aromaticity reversal in the lowest excited triplet state using a comparable set of [26]- and [28]hexaphyrins by femtosecond time-resolved infrared (IR) spectroscopy. Compared to the relatively simple IR spectra of [26]bis-rhodium hexaphyrin (R26H), those of [28]bis-rhodium hexaphyrin (R28H) show complex IR spectra in 1300-1700 cm-1 where the stretching modes of conjugated ring can be detected. On the other hand, the time-resolved IR spectra of R26H in the excited triplet state are dominated by an appearance of excited state IR absorption peaks, while those of R28H are largely composed of ground state IR bleaching peaks, which reflects the aromaticity reversal in the lowest triplet state as illustrated by the structural changes. Therefore, these contrasting IR spectral features with quantum mechanical calculations would serve as new experimental aromaticity indices showing Baird’s rule.


S_n
Intersystem Crossing
ΔT
(~ ns)
S_0
T_1
Baird Aromaticity
[4n] rule
Hückel Aromaticity
[4n+2] rule

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발표코드: **PHYS.O-2**
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 조성

The use of a local exact exchange potential enhances accuracy of hybrid DFT for excited state calculations

김재욱 김우연*

KAIST 화학과

Density functional theory (DFT) calculation has been an essential tool for electronic structure calculations. In particular, hybrid DFT method is very popular for chemistry field and computational material design because the method gives relatively accurate results in relatively small computational time compared to other electronic structure calculation methods. The conventional hybrid DFT method adopts non-local Hartree-Fock exchange operators to compensate errors of pure DFT method. Herein, we propose to use a local multiplicative potential for hybrid DFT calculations. The local version of hybrid density functionals can be derived from existing hybrid functionals by using the optimized effective potential method. In this presentation, the difference between the local and the non-local version of hybrid DFT will be demonstrated for both ground and excited state properties. We find that the time-dependent DFT calculation using the local version provides the better results for excited state than the conventional non-local one. Furthermore, the optical excitations are well described with single orbital transition due to the properties of unoccupied orbital in the local version of hybrid DFT.

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장소: 일산 KINTEX
발표코드: **PHYS.O-3**
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 09:29, 좌장: 조성

Adsorption State of Ammonia on a Crystalline Ice Surface

이두형 강헌*

서울대학교 화학부

Researchers have studied the adsorption of ammonia on ice (and water) surfaces for a long time because it has an importance in various parts of nature such as involvement in chemical reactions in atmosphere and space, but many of the details are still in a veil. Hence we investigated the ammonia adsorption state on crystalline ice Ih surfaces.Ammonia-adsorbed thin crystalline ice films were prepared on Pt(111) single crystal surface in an ultra-high vacuum environment and analyzed with surface-sensitive techniques including temperature-programmed desorption (TPD), Cs^+ reactive ion scattering (RIS), low-energy sputtering (LES), and film voltage measurement using a Kelvin workfunction probe.The ammonia desorption from crystalline ice surfaces was completed before 150 K. Also, protonated products of ammonia were not detected in the LES experiment. In the Kelvin probe measurement, ammonia adsorption changed film voltages of ice films more positive.From the desorption spectra, penetration and desorption behavior of ammonia were discussed. An analysis of the change in the film voltage showed an anisotropic distribution of ammonia molecules at ice surfaces. This directional adsorption was induced by the stronger hydrogen bonding between a nitrogen atom of ammonia molecules and a dangling hydrogen atom of ice surfaces than the bonding between hydrogen atom of ammonia molecules to a dangling oxygen atom on the ice surfaces. However, the molecules were not strictly perpendicular to the surface, but had a tilted orientation. It is inferred from the saturation of the film voltage change that the surface density of dangling H on crystalline ice surface was one fourth monolayer to the surface ice molecules, which is the same as the ideal model of crystalline ice.

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발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 09:42, 좌장: 조성

Single molecular spin crossover materials: accurate prediction of stable spin state using standard DFT

송수환 심은지*

연세대학교 화학과

In this work, we present calculations for spin-crossover (SC) compounds using a recently proposed density-corrected density functional theory (DC-DFT) method. Despite its efficiency and reasonable accuracy, density functional theory (DFT) is known to be inaccurate in problematic cases like open shell systems. In case of SC systems, DFT fails to give accurate spin states consistently and the energy difference between high spin and low spin states are inaccurate. Since controlling spin states in SC systems experimentally is extremely difficult, one needs to use computationally costly methods like coupled cluster and quantum Monte Carlo in order to predict preferred spin states. Here we show Hartree-Fock DFT (HF-DFT), one of the simplest ways to perform DC-DFT, gives prediction in spin states with accuracy comparable to coupled cluster results while its computation cost is similar to DFT. In HF-DFT, one evaluates DFT energy on HF densities which results in reducing density-driven error compared to conventional DFT calculation, and has shown promising results in open-shell systems. We believe such improvement in SC systems could be expanded to obtain correct spin-densities at no more cost than standard DFT approximations and ultimately to determine magnetization.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.O-5**
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 09:55, 좌장: 조성

Real-time Excited State Predissociation Dynamics of Thioanisole

우경철 강도형 김상규*

KAIST 화학과

Relaxation dynamics involving ππ* and nσ* excited states of thioanisole ($C_6H_5SCH_3$) in the gas phase has been investigated by picosecond time-resolved ion yield (TR-IY) and time-resolved velocity map ion imaging (TR-VMI) methods. It has been widely investigated in our group in the energy-domain [1, 2], and the striking dependence of the relative yields of two reaction channels on the photoexcitation energy was observed as indicated by a 'dynamic resonance' in the product branching ratio. Here, with our time-domain measurements, the methyl fragment rise transients were fitted well with single exponential function, except at specific excitation energy range where showing biexponential behavior with two distinct time constants. (c.f. Kinetics of CH_3^+ rise has been previously reported with fs TR-VMI method [3].) This was also confirmed by the TR-VMI experiment. This implies that two predissociating channels co-exist in the excitation energy region where S_1 and S_2 are strongly mixed, which may be correlated with the previously reported 'dynamic resonance' behavior observed from the energy-domain experiments. This result of two distinct dynamic channels should be emphasized as the first experimental observation in time-domain measurements where excited states of bound and repulsive characters are intensely coupled, which can be generalized throughout the predissociative molecules having *'Resonance-in-Continuum'* behavior.References[1] J. S. Lim, and S. K. Kim, *Nat. Chem.*, 2010, 2, 627[2] S. Han, J. S. Lim, J.-H. Yoon, J. Lee, S.-Y. Kim and S. K. Kim, *J. Chem. Phys.*, 2014, 140, 054307[3] G. M. Roberts, et al,, *Chem. Sci.*, 2013, 4, 993

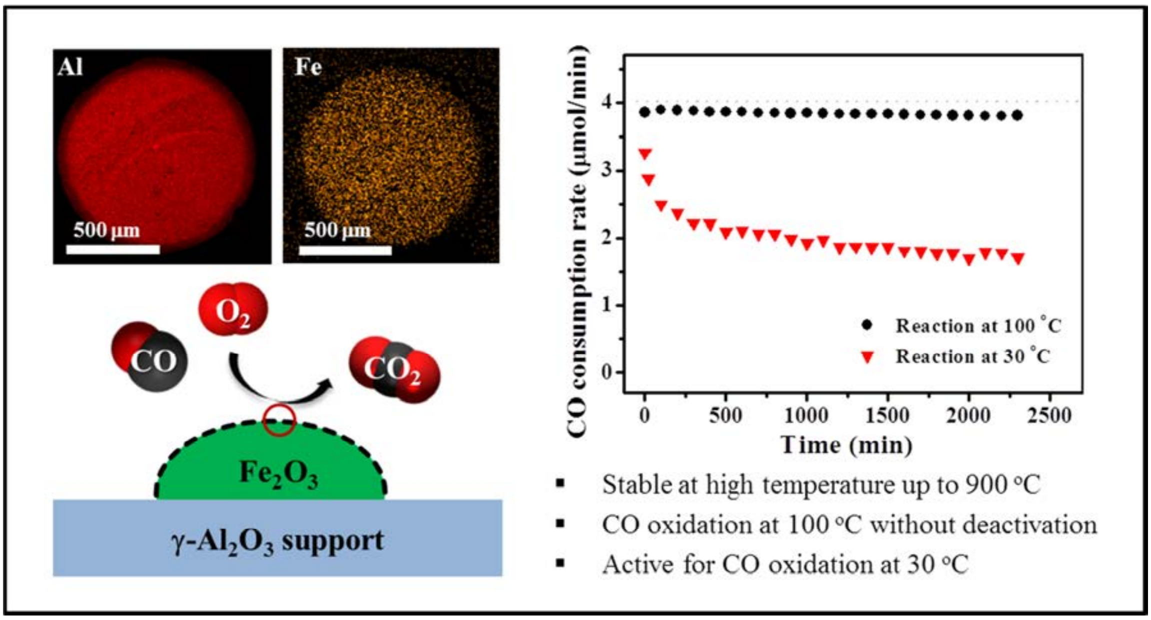
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.O-6**
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 10:08, 좌장: 조성

Low temperature CO oxidation over iron oxide nanoparticles deposited on internal structures of mesoporous alumina bead: deactivation-free catalysts at ~ 100 ^{o}C

김일희 한상욱 박찬흠 정재환 김호종 차병준 우태균 김영독[*] 서현욱[1,*]

성균관대학교 화학과 [1]상명대학교 화학에너지공학과

By a chemical vapor deposition method with regulating temperature of reactor under ambient pressure conditions (temperature regulated-chemical vapor deposition, TR-CVD), we were able to decorate the internal structure of a mesoporous Al_2O_3 bead (particle size of ~ 1 mm, Sasol) with iron oxide nanoparticles (with a mean lateral size of ~ 1 nm). The iron oxide-decorated Al_2O_3 showed a high catalytic activity for CO oxidation even at room temperature. Subtle deactivation of the CO oxidation activity was observed with increasing reaction time at ~ 100 ^{o}C. Additionally, the catalyst maintained the catalytic activity even after severe thermal treatment at ~ 900 ^{o}C, under ambient conditions. We show that our catalysts prepared by TR-CVD have potential for application as oxidation catalysts in industrial process due to the simplicity of their fabrication process as well as the high and stable catalytic performance.



- Stable at high temperature up to 900 °C
- CO oxidation at 100 °C without deactivation
- Active for CO oxidation at 30 °C

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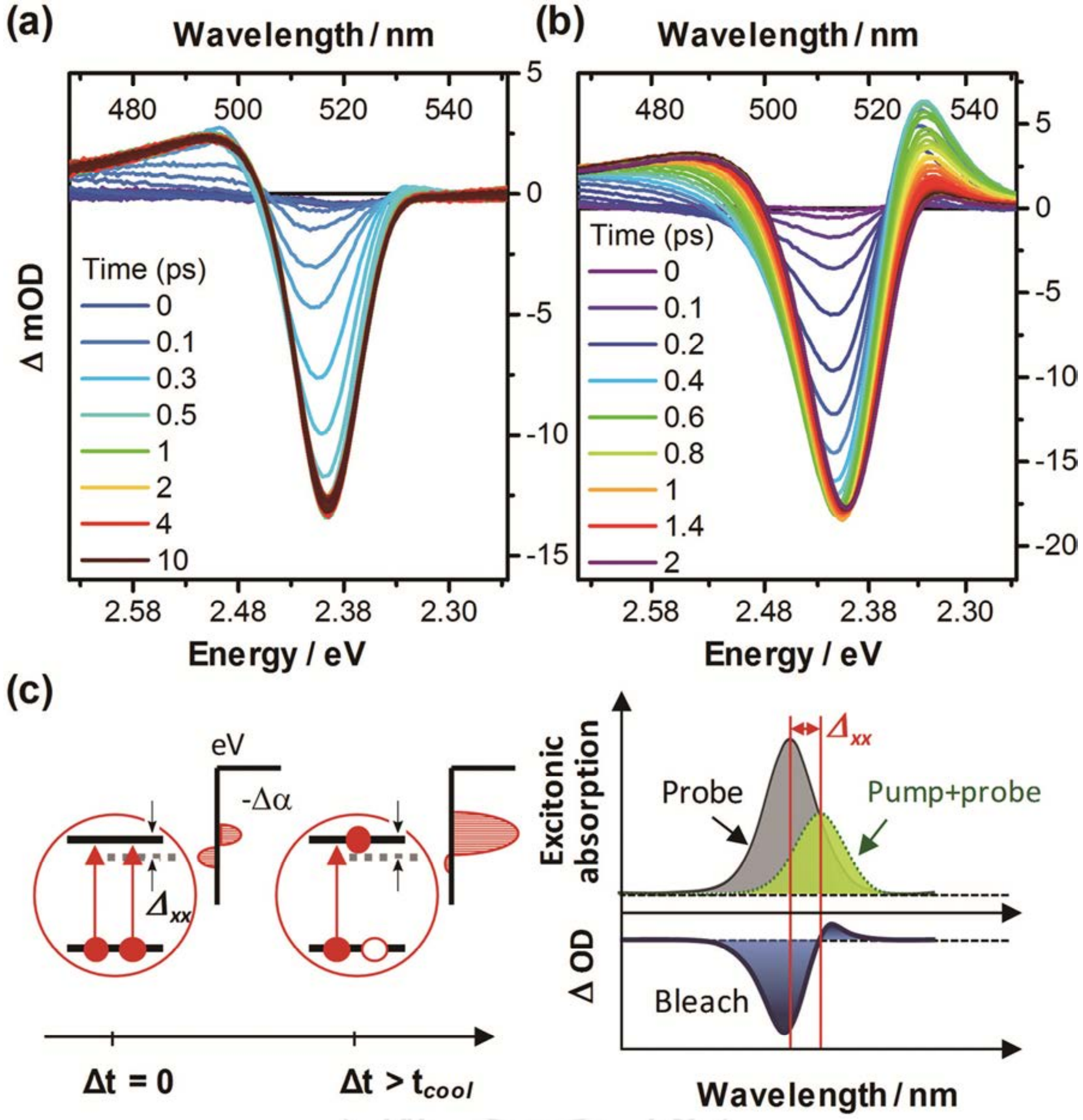
장소: 일산 KINTEX
발표코드: **PHYS.O-7**
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 10:21, 좌장: 조성

Composition-dependent Hot Carrier Relaxation Dynamics in Cesium Lead Halide (CsPbX3, X= Br and I) Perovskites Nanocrystals

정희재 김효진 심은지 김동호*

연세대학교 화학과

Cesium-based perovskites nanocrystals (NCs) have outstanding photophysical properties (e.g. narrow-band photoluminescence and high quantum yields) improving the performances of lighting devices. Fundamental studies on excitonic properties and hot-carrier dynamics in perovskite NCs further suggest that these materials show higher efficiencies compared to the bulk form of perovskites. However, the relaxation rates and pathways of hot-carriers are still being elucidated. One of the most relevant mechanisms of intraband hot-carrier relaxation is thermalization process coupled with lattice vibrations. By using ultrafast transient spectroscopy and calculating electronic band structures, we investigated the dependence of halide in Cs-based perovskites (CsPbX3 with X = Br, I, or their mixtures) NCs on the hot-carrier relaxation processes. All samples exhibit ultrafast (< 0.6 ps) hot-carrier relaxation dynamics with following order: CsPbBr3 (310 fs) > CsPbBr1.5I1.5 (380 fs) > CsPbI3 NC (580 fs). These result accounts for a reduced light emission efficiency of CsPbI3 NC compared to CsPbBr3 NC.


(a)
Wavelength / nm
480
500
520
540
5
0
-5
-10
-15
Δ mOD
Time (ps)
0
0.1
0.3
0.5
1
2
4
10
2.58
2.48
2.38
2.30
Energy / eV
(b)
Wavelength / nm
480
500
520
540
5
0
-5
-10
-15
-20
Time (ps)
0
0.1
0.2
0.4
0.6
0.8
1
1.4
2
2.58
2.48
2.38
2.30
Energy / eV
(c)
eV
-Δα
Δ_{xx}
Δt = 0
Δt > t_{cool}
Excitonic absorption
Δ_{xx}
Probe
Pump+probe
Δ OD
Bleach
Wavelength / nm

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.O-8**

발표분야: Oral Presentation for Young Scholars in Physical Chemistry

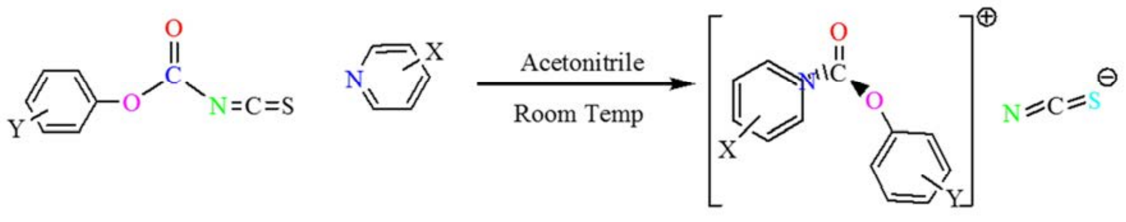
발표종류: 구두발표, 발표일시: 목 10:34, 좌장: 조성

CPCM Study on the Pyridinolysis of Phenyl Carbonyl Isothiocyanate in the Gas and Acetonitrile Solvent

Adhikary Keshab Kumar 김찬경*

인하대학교 화학과

Experimentally, the nucleophilic substitution to the carbon center could proceed through two different mechanisms: concerted or stepwise. Our present study focuses on the mutual interaction of the substituents in the nucleophile and substrate. The concerted single step substitution reaction shows a small negative ρ_{XY} value. In this work (Scheme 1), the reaction mechanism on the pyridinolysis of phenyl carbonyl isothiocyanates is investigated in the gas phase and acetonitrile solvent using the CPCM approach at the B3LYP/6-311+G(d,p) level of theory. We optimized all the reactant complexes, transition states, and product complexes to construct the potential energy surfaces (PES) for six different substituents and confirmed by frequency calculations. The reaction mechanism is discussed with Hammett constants, ρ_X, ρ_Y, β_X, cross interaction constant (CIC) ρ_{XY}, NBO charges and structure-energy relationships. Orbital interactions and the stereo-electronic effect between the nucleophile and the substrate are also considered to confirm the reaction mechanism.



X = 4-MeO (1), 4-Me (2), H (3), 3-Cl (4), 4-Ac (5), 4-CN (6)
Y = 4-MeO (1), 4-Me (2), H (3), 3-MeO (4), 4-Cl (5), 4-CN (6)

Scheme 1. Reaction scheme studied in this work.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.O-9**
발표분야: Oral Presentation for Young Scholars in Physical Chemistry
발표종류: 구두발표, 발표일시: 목 10:47, 좌장: 조성

Full Characterization of Ultrafast Excited-State Intramolecular Proton Transfer with Sub-10 fs Two-Color Transient Absorption Experiment

김준우 주태하*

POSTECH 화학과

Excited-state intramolecular proton transfer (ESIPT) is a photo-induced tautomerization between the enol and keto form of the molecule. In general, ESIPT is has relatively faster reaction rate and larger Stokes shift than other photo-induced reactions. Because of these unique properties of ESIPT, it is applied for various fields, such as white light source, LED, molecular probe. Understanding of ESIPT dynamics can improve or modify its applications. Despite of its uniquity, its excited-state dynamics is not well understood by chemists. One main reason of that is the difficulty on studying a specific excited-state dynamics occurring in condensed phase. It is difficult to observe a specific dynamics, where it always accompanies other dynamics. In order to prevent the other dynamics interferes the observation of ESIPT, the system should have small and rigid structure and small charge transfer character in the excitation. In this research, 10-hydroxy[h]benzoquinoline (HBQ), which is well known for an ultrafast ESIPT system, is investigated as the fundamental study of ESIPT, where HBQ satisfies the conditions listed above. The excited-state dynamics of HBQ was measured with a NUV pump / visible continuum probe transient absorption (TA) apparatus, whose time resolution is sub 10 fs. By virtue of the high resolution, the Frank-Condon excitation induced vibrational spectrum (FEVS) of HBQ could be measured to 3000 cm-1. Since FEVS can be simulated by a simple quantum mechanical calculation, we compared the experimental and theoretical FEVS of HBQ and several important properties, such as electronic and nuclear structure, of HBQ can be obtained to conclude what are important factors in ESIPT.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-1**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 하지원

Analysis of Alzheimer’s Disease Biomarkers in Blood Samples using Surface Plasmon Resonance

김수희 이혜진[1,*]

경북대학교 자연과학대학/화학과 [1]경북대학교 화학과

본 발표에서는 혈액 샘플에서 알츠하이머 질병 진단 바이오마커 검출을 위한 새로운 표면 샌드위치 분석법을 보여주고자 한다. 알츠하이머 질병 진단 바이오마커 중 대표적인 물질인 alpha-1 antitrypin(AAT)1 과 tau2 단백질을 압타머/바이오마커/항체의 표면 샌드위치 복합체를 형성하여 surface plasmon resonance (SPR)로 검출하고자 하였다. 또한 실제 샘플에 존재하는 AAT 와 tau 단백질을 정량적으로 검출하기 위하여 비특이적 흡착 반응에 의한 SPR 신호를 줄이기 위한 블로킹표면화학을 도입하였다. 그 결과, 혈액 내에 존재하는 AAT 와 tau 단백질을 약 fM 까지 검출할 수 있음을 확인할 수 있다.References(1)Kim, S.; Lee, H. J. Anal. Chem., 2015, 87, 7235-7240.(2)Kim, S.; Wark, A. W.; Lee, H. J. Anal. Chem., 2016, 88, 7793-7799.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-2**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:10, 좌장: 하지원

Hydrogel Microparticle for Highly Selective and Sensitive RT-qPCR

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Reverse transcription – polymerase chain reaction (RT-qPCR) is commonly used method to analyze oncogenes, infected DNAs, and mutated tumor associated genes. However it is hard to detect rare genetic targets since the disturbance of undesired amplification often overrides the reaction of very few targets in a myriad of interfering genes. Previously, we developed primer-immobilized network (PIN) - based RT-qPCR. PIN-based RT qPCR can capture target RNA with immobilized primers. Moreover, non-target RNA can be washed out by washing process. However, still false-positive signal was occasionally appeared in negative cases so that it can make wrong decision in clinical cases. To overcome this limitation, we improved washing protocol borrowed from a method conventionally used in a microarray. Furthermore, we established TaqMan probe-based assay instead of SYBR Green Ⅰ. We confirm that cycle threshold value (Ct value) was clearly decreased from 32 to 39~40 in negative cases. That means most non-target RNAs and interfering substances were washed away. Also, TaqMan probe-based qPCR can detect single-copy of template in a PIN particle with more than 90% of PCR efficiency. Owing to these process, PIN-based RT-qPCR can detect rare target in tens of pico grams of total RNAs. This advanced PIN RT-qPCR will soon be validated with rare target gene in clinical samples.

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Keywords: Hydrogel microparticle, Rare mutation, Reverse transcription, Real-time polymerase chain reaction

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-3**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 하지원

Single Particle Study on Size-dependent Optical Properties of Gold Nanospheres beyond the Quasi-Static Limit

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울산대학교 화학과

Gustav Mie solved Maxwell's equations to account for the absorption and scattering of spherical plasmonic particles in 1908. Since then much efforts have been devoted to the size dependent optical properties of gold nanoparticles. However, our understanding of the dark-field (DF) scattering properties of single gold nanospheres (AuNSs) beyond the quasi-static limit is still limited, and there have been no studies to elucidate their optical properties under differential interference contrast (DIC) microscopy. We therefore employed single particle DF and DIC microscopy to investigate the particle size dependency for AuNSs with different diameters from 100 nm to 400 nm beyond the quasi-static limit. We found that higher order plasmon resonances are observed in the single particle scattering spectra of large AuNSs (300 nm and 400 nm). Furthermore, the DF and DIC intensities were linearly increased as the particle size was varied from 100 nm to 400 nm. Therefore, the results provide useful experimental information about how the optical properties evolve with the particle size for designing the optimal plasmonic AuNSs or nanostructures in a particular use.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-4**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:22, 좌장: 하지원

Characterizing the Optical Properties of Single Gold bipyramids with Sharp Tips as Single Particle Orientation Probes

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울산대학교 화학과

Plasmonics metallic nanoparticles have a potential for various applications in optics, catalysis, sensor, medicine etc. Recently, single metallic nanoparticles are gaining much attention as an attractive biomolecular sensor. Especially, gold bipyramids are expected to be a promising material for biosensors to obtain high detection sensitivity due to its sharper tips compared with spherical gold nanoparticle or rod-shape gold nanoparticle and present high scattering cross-section. Herein, we performed single particle study to characterize the optical properties of gold bipyramids with sharp tips under scattering-based dark-field (DF) and differential interference contrast (DIC) microscopy, and to examine their use as orientation probes in biological and physical studies. We found polarization-dependent DIC images and intensities of single gold bipyramids, which enabled for the determination of their orientation angle under DIC microscopy. Furthermore, we found that DIC polarization anisotropy can be obtained from the orthogonally polarized bright and dark intensities for more accurate and reliable angle measurements of single gold bipyramids.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-5**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 09:24, 좌장: 하지원

Three-dimensional Defocused Orientation Sensing of Single Bimetallic Core-Shell Gold Nanorods as Multifunctional Optical Probes

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울산대학교 화학과

Bimetallic core-shell gold nanorods (AuNRs) are promising multifunctional orientation probes that can be employed in biological and physical studies. This paper presents the optical properties of single AuNRs coated with palladium (Pd) and platinum (Pt) under scattering-based dark-field (DF) microscopy. Strong longitudinal plasmon damping was observed for the bimetallic AuNRs due to Pd and Pt metals on the AuNR surface. Despite the strong plasmon damping, the bimetallic AuNRs yielded characteristic doughnut-shaped scattering patterns under defocused DF microscopy. Interestingly, a solid bright spot appeared at the center of the defocused scattering patterns due to strong damping in the longitudinal plasmon and the increased contribution from the transverse dipoles to the image patterns, which was verified further by a simulation study. Furthermore, the defocused scattering field distributions enabled a determination of the three-dimensional (3D) orientations of single bimetallic AuNRs through a pattern-match analysis technique without angular degeneracy. Therefore, deeper insight into the optical properties and defocused scattering patterns of single bimetallic AuNRs is provided, which can be used to develop multifunctional optical probes that are capable of sensing of the 3D orientation of a probe, biomolecules based on LSPR shift, gas and humidity, etc.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-6**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:26, 좌장: 하지원

[발표취소] Direct Screening of H7N9 Virus DNA based on Spectral Imaging without Target Amplification

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경희대학교 응용화학과

발 표 취 소
본 논문은 발표취소된 논문입니다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-7**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:28, 좌장: 하지원

Super-Localization of Immunoplasmonic Particle for Ultra-Sensitive Detection of Alpha-Fetoprotein on Nanobiosensor by Scattering-Based Super-Resolution Microscopy

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경희대학교 일반대학원 화학과 [1]경희대학교 응용화학과

Immunoplasmonic particles were super-localized within highly specific region for sensitive detection of alpha-fetoprotein (AFP) with total internal reflection scattering super-resolution microscopy (TIRS-SRM). 20-nm silver nanoparticles were used as a nanoprobe to detect AFP molecules and 100-nm gold nanoisland (GNI, substrate) were selected as a substrate. Individual scattering signals and images of immunoplasmonic particle and GNI were acquired within evanescent field layer by TIRS-SRM using 405 nm and 635 nm illumination, respectively. The center coordinates of the Immunoplasmonic particles were determined within highly specific region (GNI) by applying 2D Gaussian fitting to point spread function. Limit of detection (LOD) of the developed method was 7.04 zM, which was at least 100 times lower than LODs obtained with the previously reports. The TIRS-SRM was demonstrated to be an effective tool to localize individual protein molecules within specific regions for distinguishing each signal and sensitive detection. The method was reliable and effective detection of disease-related protein molecules as diagnostics.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-8**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 하지원

Immunoreaction-based dual-wavelength capillary electrophoresis for simultaneous detection of thyroid hormones

우나인 강성호[1,*]

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Immunoreaction-based capillary electrophoresis (CE) with a laser-induced fluorescence (LIF) detector was developed for the fast and highly sensitive detection of thyroid hormones. Thyroid hormones have been reported to influence various diseases such as hypothyroid, hyperthyroid, thyroidectomy, and thyroiditis. Therefore, measurements of T4, T3, and TSH are useful for the clinical evaluation of thyroid function. In this study, immunoreaction and biotin-streptavidin interaction were investigated for highly sensitive detection of thyroid hormones as a function of migration time and separation efficiency. Various factors such as the effective length, separation voltage, and pH of running buffer were also examined in order to determine the optimal CE conditions. All three standard thyroid hormones were analyzed within 3.2 min in 25 μM $Na_2B_4O_7$-NaOH buffer (pH 9.3) without losing resolution under optimum conditions, which were 1,000-100,000 times more sensitive than other previous detection methods. In addition, the CE with LIF detection method also successfully applied to the analysis of real human blood samples. Consequently, the immunoreaction-based CE method with LIF detection is an effective, rapid analysis technique for highly sensitive detection of thyroid hormones related to thyroid gland disease.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-9**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 09:32, 좌장: 하지원

Real-Time In-Situ Nano-Carrier Quantification by Super-Resolution Microscopy in Live Single Cells

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경희대학교 화학과 [1]경희대학교 응용화학과

The extent of time-dependent subdiffraction-limit super-resolution imaging in single molecule tracking and localization has been a great asset in the biomedical field. Quantifying and assessing drug/gene-carrying nanoparticles at the cellular level was crucial in visualizing the nano-toxicity to hold good for drug delivering applications. In this work, a 50 nm drug carrier containing rhodamine B isothiocyanate dye was quantified, tracked, and assessed toxicity at HEK293, NIH3T3, and RAW 264.7 cells using direct stochastic optical reconstruction microscopy (*d*STORM). Results suggest that the RAW 264.7 cells possess higher uptake efficiency of nano-carrier than HEK293 and NIH3T3 cells. Moreover, the nano-carrier was observed to break the biological barrier to be internalized within the nuclei of RAW 264.7 and HEK293 cells. Additionally, the micronuclei were detected more in RAW 264.7 cells than in other two cells suggesting disruption in usual chromosomal DNA breakage. A first ever combined approach of *d*STORM, transcriptomics, and molecular biology paid way for assessing nano-carrier in three different cells at specific sites with precise sensitivity. The subdiffraction-limit super-resolution microscopy *d*STORM resolves quantitative differences in the uptake efficiency of nano-carrier and assess internalized nano-carrier locality in live single cell.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-10**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:34, 좌장: 하지원

NMR study of Arginine ε-NH NMR Signal Assignment in Human Cytosolic Adenylate Kinase 1

김길훈 원호식*

한양대학교 응용화학과

In many of nucleotide binding proteins, Arg residues are known to play important roles in substrate binding through the electrostatic interaction of positive charge on the Arg side chain with the negative charge of phosphoryl group. Adenylate kinase1(AK1) has some Arg residues necessary for binding its substrates, MgATP, AMP. To investigate the interactions between Arg side chains and the substrate in aqueous solution, we observed the signals of Arg ε-NHs of ^{15}N-labeled AK using ^{1}H, ^{15}N two dimensional NMR. The experiments with HSQC pulse sequence detected 13 signals corresponding to all Arg residues on human cytosolic AK1(hAK1). In NMR spectra, we used single quantum coherence SQC as pulse sequence, only the ε-NH signal on Arg side chain can be detected in the specific resonance region. These signals are good markers to study the inter actions between the substrate and proteins with high molecular weight. However, this process is often hard to assign near the terminus of the long side chain such as Arg residues. Therefore, we focused of on six conserved Arg and assigned only these signals by comparison with the spectra of each Arg mutant. The 6 signals derived from 6 Arg residues conserve beyond species (Arg[44], [97], [128], [132], [138], and [149]) were assigned using each mutants which substituted by Ala residue (R44A, R97A, R128A, R132A, R138A and R149A). This method had the problem that the structural perturbation induced by the substitution of amino acid would make the assignment impossible. In the spectra of R44A, R97A, and R128A mutants, there were few problems. Although some perturbations appeared by occurred in R132A, R138A, and R149A of AK1 mutants, the consideration of the assignment for the other signals permitted these signal to be assigned.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-11**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:36, 좌장: 하지원

Substrate Binding Studies of Human Cytosolic Adenylate Kinase1 by NMR

김길훈 원호식*

한양대학교 응용화학과

Arginine residues are known to play important roles in substrate binding through the electrostatic interaction of positive charge on the Arg side chain with the negative charge of phosphoryl group in many of nucleotide binding proteins. Human cytosolic adenylate kinase1(hAK1) has some Arg residues necessary for binding its substrates including MgATP and AMP. To investigate the interactions between Arg side chains and the substrate in aqueous solution, we observed the signals of Arg ε-NHs of ^{15}N-labeled AK using ^{1}H, ^{15}N two dimensional NMR. The experiments with SQC pulse sequence detected 13 signals corresponding to all Arg residues on hAK1(human cytosolic AK1). The 6 residue signals (Arg[44], [97], [128], [132], [138], and [149]) playing important roles in substrate binding associated with LID and AMP binding domain out of all corresponding 13 Arg residues were selectively assigned through Arg to Ala substitution. In kinetic studies, the resulting large increases in the $K_{m,app}$ values for AMP^{2-} of the mutant enzymes, the relatively small increases in the $K_{m,app}$ values for $MgATP^{2-}$, and the fact that the R132A, R138A, and R149A mutant enzymes proved to be very poor catalysts are consistent with the idea that the assigned substrate binding sites. Two substrates, MgATP and AMP were titrated into wild type hAK1 and mutants to observe the effects on these assigned signals. The addition of AMP affected 4 Arg signals, whose chemical shift took place a down field in the direction on proton dimension whereas the addition of MgATP did few effects. We were able to find that the Arg[44] specifically interact with the phosphoryl group of AMP. The additions of both the substrates augmented significantly the intensity of Arg[149] signal, which had very low intensity on the spectrum of free wild type AK1. Three ε-NH signals derived from Arg[123], [132], and [138] were broadened and disappeared upon the Mg-ATP addition. These arginine residues locate on α-helix and the following loop along the moiety of triphosphate of MgATP.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-12**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:38, 좌장: 하지원

Supersensitive Plasmonic Single Nanoparticle-based Cancer Antigen 125 Immunodetection by Dual-Mode Wavelength-Dependent Enhanced Dark-Field Microscopy

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A supersensitive immunodetection was achieved for the biomarker cancer antigen 125 (CA125), which was developed based on characterization of single-particle plasmonic scattering by dual-mode wavelength-dependent enhanced dark-field microscopy (EDFM-DM). For simultaneous dual-detection, an electron multiplying cooled charge-coupled device camera and color digital camera were used for qualitative and quantitative analysis, respectively, based on the dark-field scattering images. To prove the efficacy of EDFM-DM for the dectection of scattering signals, various size of different plasmon nanoparticles (i.e., gold nanoparticles, 5 nm, 12 nm, 20 nm, 100 nm and 250 nm; silver nanoparticles, 20 nm, 30 nm, 40 nm, 80 nm and 100 nm) were used as the detection tags and investigated with wavelength dependence of the light source, and the quantum efficiency of the electron-multiplying charge-coupled device camera, 40-nm silver nanoparticle (AgNP) was selected as an optimum fluorescence-free probe. CA125 ovarian cancer antigen was screened at single-molecule level and quantitatively analyzed by measuring the scattering signals of 40-nm AgNP on gold-nanodots arraychip with lowest possible LOD (4 μU/mL, $S/N = 3$) with a wide dynamic detection range of 4 μU/mL-80 U/mL ($R = 0.9935$), which was a 100-375,000-fold lower detection limit with a 100-100,000-fold wider dynamic range than previous detection methods. In addition, recovery was greater than 98% with the spiking of standard CA125 in human serum samples. Dual-mode EDFM-DM based optical property of the plasmon nanoparticle allowed us for a sensitive detection of disease related biomolecules at single-molecule level.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-13**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:40, 좌장: 하지원

Platinum-coated Core-Shell Gold Nanorods as Multifunctional Orientation Sensors in Differential Interference Contrast Microscopy

이준호 김근완 하지원*

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We characterized optical properties of single platinum-coated core-shell gold nanorods (Pt-AuNRs) under dark-field (DF) and differential interference contrast (DIC) microscopy. Furthermore, we examined their potential use as multifunctional orientation probes. The longitudinal surface plasmon resonance damping is observed for single Pt-AuNRs due to Pt metals coated on the AuNR surface under single particle scattering spectroscopy. Despite the strong plasmon damping with much decreased scattering intensity, DIC microscopy allowed us to detect single Pt-AuNRs with much higher sensitivity. We found polarization-dependent DIC images and intensities of single Pt-AuNRs, which allows us to determine their orientation angle under DIC microscopy.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-14**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:42, 좌장: 하지원

Metabolic alteration induced by IDH1 R132H mutant of glioma revealed by LC-MS/MS

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Glioma is a type of brain tumor originating from tissues that bind and nourish neural tissue inside the brain and spinal cord. Most patients who are diagnosed with glioblastoma, the most common type of glioma have a median survival rate only for about 14 months, and only 3 to 5 percent of the patients are known to survive for more than 5 years [1][2]. Recently the R132H mutation of isocitrate dehydrogenase 1 (IDH1) were discovered in glioblastomas [3]. IDH1 is a metabolic enzyme that catalyzes the oxidative decarboxylation of isocitrate, producing alpha-ketoglutarate in the cytosol [4]. However, the IDH1 R132H mutant enzyme converts isocitrate to 2-hydroxyglutarate (2HG) instead that leads to a hypermethylated state of DNA and histones altering different gene expression in glioma [5]. The goal of this study is to quantitatively survey the metabolic profiles between normal IDH1 and mutant IDH1 R132H by LC-MS/MS. We found that a number of metabolites related to major metabolic pathways were altered with the IDH1 R132H mutation in glioma. This result can be used to find potential targets in glioma with the IDH1 R132H mutation. We expect that the comprehensive understanding of metabolic alteration induced by IDH1 R132H mutant of glioma may help the development of inhibitory drugs that may rectify the altered metabolic pathways by 2HG.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-15**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:44, 좌장: 하지원

Circulating Biomarker Database (CBD), A Comprehensive Transition Database for LC-MS/MS Based Screening for FDA-approved Biomarkers in Blood

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Biomarkers are a type of biological molecules that are objective indications of medical state which can be measured accurately and reproducibly.[1] Currently, there are thousands of biomarker tests approved by FDA and only a few are being measured when a clinical concern is raised by medical doctors. Although the early diagnosis can be done by monitoring them regularly, there is no FDA-approved method to carry out the routine measurement of these biomarkers in a global fashion. Recent advance in high resolution mass spectrometry can now allow a clinical laboratory to measure analytes of interest from specimen very accurately and reproducibly.[2] Especially, the targeted mass spectrometry such as MRM (multiple reaction monitoring) has the potential to be the major technology to monitor these thousands of biomarkers in a clinical setting. In this regards, we create a database called Circulating Biomarker Database (CBD) as the first step which is a comprehensive transition list for LC-MS/MS-based screening of FDA-approved biomarkers. In this database, precursor ions of 583 biomarkers and their fragment ions as transitions are listed together towards a comprehensive monitoring method to screen most biomarkers in blood. In conclusion, Circulating Biomarker Database can be used for clinical diagnostics and prognostics in the future medicine.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-16**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:46, 좌장: 하지원

Enhanced quantification of phospholipids using isotope-labeled methylation using nUPLC-ESI-MS/MS

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Phospholipid (PL) is one of the most important type among various lipid classes in biological cells. Quantitative analysis of PLs is crucial as they regulate several important functions such as formation of cell membrane, intercellular signaling, and energy storage. Conventionally, lipid quantitation using LC-MS is often carried out with the addition of internal standards to compensate the ionization fluctuation. However, the use of internal standards is limited by several reasons; lipid standards of various molecular structures are limited and accurate determination of lipid amount is difficult. In this study, a quantitative analysis of PLs was accomplished, based on an isotope-labeled methylation (ILM) method using (trimethylsilyl)diazomethane as a methylation reagent to methylate the phosphate or carboxyl group. MeOH and HCl were utilized for light isotope-labeled methylation, while MeOD and DCl containing deuterium were used for counterpart methylation. ILM method was validated concerning efficiency of methylation, optimization of modifiers, and peak area linear relationship of H- and D- labeled methylated lipids. This method consequently applied to DU145 cell line with and without D-allose treatment. In the end, a total of 112 PLs including LPG, PG, LPS, PS, LPA, PA, and CL were identified. Among these lipids, 8 and 25 more PAs and CLs, respectively, were detected from ILM method, when they were not detected in intact lipid extracts.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-17**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:48, 좌장: 하지원

Top-down proteomic analysis of HDL from coronary artery disease patients using flow field-flow fractionation and mass spectrometry

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Coronary artery diseases (CAD) refers to a condition in which coronary arteries become narrow by accumulation of cholesterols, fats, and other substances. Narrow arteries restrict blood flow to heart and may even cause a partial or complete blockage of arteries. High-density lipoprotein (HDL) has been reported to be associated with CAD of which few marker proteins are of interests. HDL is composed of various lipids and proteins including apolipoproteins and recent studies have reported that apolipoprotein A-I (apo A-1) in HDL undergoes oxidation during the development of CAD. As other types of proteins in HDL are highly likely to undergo changes, analysis of HDL-related proteins is necessary to understand the relationship between HDL and CAD more effectively. Flow field-flow fractionation (FlFFF) is a separation technique based on size in a range of nano to micrometer and in this study, FlFFF was applied to separate the HDL from human plasma of CAD patients. A miniaturized asymmetrical FlFFF (AF4) channel was coupled on-line to electrospray ionization mass spectrometry (ESI-MS) for a high speed separation of lipoproteins and top-down proteomic analysis in order to investigate the perturbation in HDL-related proteins due to development of CAD.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-18**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 하지원

Evaluation of risk factors for non-alcoholic fatty liver disease using nanoflow UPLC-ESI-MS/MS

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Non-alcoholic fatty liver disease (NAFLD) is one of the most frequent cause of deaths worldwide, associated with obesity and insulin resistance due to unhealthy lifestyle. With excessive amount of fat accumulated on liver tissue, a spectrum of NAFLD encompasses a wide range of conditions ranging from simple steatosis to advanced cirrhosis. As a number of factors such as high cholesterol diet and inflammation are possible risk factors of NAFLD, the effect of various risk factors on hepatic lipid metabolism was evaluated in this study using nanoflow ultrahigh-pressure liquid chromatography electrospray-ionization tandem mass spectrometry (nUPLC-ESI-MS/MS). Lipids from hepatic tissue from rabbits grown under the conditions of healthy diet (C), inflammation by injecting carrageenan (I), high cholesterol diet (HC), and high cholesterol diet with inflammation by injecting carrageenan (HCI) were structurally identified based on collision-induced dissociation (CID) spectra obtained from nUPLC coupled with ion trap MS, followed by a targeted quantification of the identified lipids using nUPLC coupled with triple quadrupole MS in selective reaction monitoring (SRM) mode. Over 300 hepatic phospholipids, sphingolipids, and glycerols were analyzed and significant and dramatic changes were observed from HC and HCI groups but not I, indicating that intake of high cholesterol food altered hepatic lipidome significantly while inflammation did not.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-19**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 09:52, 좌장: 하지원

Effect of cationic monomer composition on polymerization of cationic polyacrylamide copolymers using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

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Cationic polyacrylamide (CPAM) copolymers are often used as flocculants in wastewater treatment and they have high molecular weight distribution (~108 g/mol) and viscosity. Physicochemical properties of CPAM depend on polymerization methods (solution polymerization and emulsion polymerization), chain types (linear and branched), cationic monomer composition, and amount of cross-linking agent. In this study, influence of these factors on molecular weight distribution and conformation of CPAM copolymers was evaluated using an elution-based separation technique, flow field-flow fractionation (FlFFF), and multi-angle light scattering- differential refractive index (MALS-DRI). In terms of cationic monomer composition, CPAM tended to become more compact with increased molecular weight distribution when cationic monomer composition was increased in solution polymerization and in emulsion polymerization, CPAM seemed to be aggregated when cationic monomer composition was less than 10 mol%. When the amount of cross-linking agent was increased, CPAM tended to be synthesized smaller and more compactly. Also, FlFFF is operated in either normal or steric/hyperlayer mode depending on the size of sample particles and in this study, a transition between two different modes of separation was observed under gradient elution.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-20**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:54, 좌장: 하지원

Analysis of prostate cancer-derived urinary exosomes by flow field-flow fractionation

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Exosomes are extracellular vesicles with 20 to 100 nm in diameters and they are involved in intercellular communication by transporting biomolecules such as mRNA, proteins, and lipids. They exist in all kinds of body fluids including urine and blood. Recently, research on exosomes of body fluids has emerged as a crucial component in biomedical field as exosomes are reportedly potential biomarker candidates of many diseases. Among various types of exosomes, urinary exosomes are closely associated with a development of prostate cancer (PCa) and their sizes are different compared to healthy controls. Flow field-flow fractionation (FlFFF) was used in this study to fractionate urinary exosomes by their size. FlFFF is an elution-based method for separating sample components according to size by an increasing order of hydrodynamic diameters and as raw samples can be directly injected into an empty FlFFF channel, the separated sample components can be collected in their intact forms, which is one of a great advantage of using FlFFF. In this study, urinary exosomes from healthy controls and PCa patients, which were first isolated from fresh urine samples by ultracentrifugation, were separated by FlFFF and clear difference in size distribution between two groups was observed. Furthermore, size-separated urinary exosomes were collected for lipidomic analysis using nUPLC-ESI-MS/MS and different lipidomic profiles and variations from large- and small-sized exosomes were observed between the groups.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-21**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:56, 좌장: 하지원

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

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Lipoproteins are carrier molecules that transport lipids and cholesterol in the bloodstream. Low levels of high-density lipoprotein (HDL) and high levels of low-density lipoprotein (LDL) in plasma are known to be related with the development of various types of diseases. Therefore, it is important to study lipoproteins at the molecular level to understand its metabolism and relationship to disease progression. Alzheimer’s disease is the most common form of dementia worldwide, taking up around seventy percent of dementia cases. A beta-amyloid, a cause of Alzheimer’s disease, is a toxic protein that kills brain neurons as its number increases. As a few studies have reported that beta-amyloid accumulates when HDL is low and LDL is high in plasma, a separate profiling of lipids from HDL and LDL is necessary to understand how the lipid metabolism within each class of lipoprotein is altered when Alzheimer’s developed.In this study, HDL and LDL from of pooled plasma samples of human controls, patients with mild cognition impairment, and Alzheimer’s disease patients were fractionated by asymmetrical flow-field flow fractionation (AF4) and lipids from the collected fractions of HDL and LDL were extracted. Using nanoflow ultrahigh-pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUPLC-ESI-MS/MS), the extracted lipids were structurally identified based on collision-induced dissociation for qualitative analysis and the identified lipids are going to be selectively quantified to evaluate the difference between three groups.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-22**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 09:58, 좌장: 하지원

NMR Structural studies associated with the mechanism of Syndecan-4 Receptor

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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. Syndecan-4 interacts with various binding partners to increase wound healing, cell invasion and survival, activates focal adhesion and phosphorylates, and regulate cytoplasmic calcium concentration. In addition, the interaction of syndecan-4 with GFRs (growth factor receptors) is a very important factor in cancer progression and is particularly associated with resistance to treatment and therapy in breast cancer.To get a better understanding of the mechanism and function of syndecan-4, it is crucial to investigate its three dimensional structure. Syndecan-4 comprises three major sections: extracellular (ecto-), transmembrane (TM) and cytoplasmic (Cyto-) domains. Syndecans have a very well conserved cytoplasmic region, but the V regions have a distinctive feature for each syndecan family member. The cytoplasmic domain of syndecan-4 consists of 28 amino acids and includes V domain. The binding of PIP2(phosphotidylinositol (4,5)-bisphosphate) 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-). And its structure was investigated by solution/solid-state NMR spectroscopy.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-23**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 하지원

3D topological studies of antimicrobial peptides with enhanced activities derived from Lactophoricin

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Since wide spread of antibiotic resistance bacterial pathogens have been prevalent it is important to investigate 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 of 11 were designed and modified to enhance antibacterial activity using conservative sequence change. Three peptides were selected among LPcin analogs via results of bacterial killing and growth inhibition assays. 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. 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. And we will also present the optimized design, construction, and good efficiency of a home-built 800 MHz (NB) narrow-bore 1H-15N solid-state NMR probe for solid-state NMR studies of antimicrobial peptides.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-24**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:02, 좌장: 하지원

The structural characterization of disease related human transmembrane proteins using the NMR spectroscopy

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Transmembrane proteins play critical roles in biological processes such as 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 transmembrane domain from human amyloid beta protein (hAβ-TM) and second transmembrane domain from human melanocortin-4 receptor (hMC4R-TM2). The hAβ-TM shows membrane-bound oligomeric state, and the Ca2+-permeable ion channel formation of non-fibrillar state in the cell membrane. So these channels can disrupt the normal cellular calcium homeostasis. It causes 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 hAβ-TM and hMC4R-TM2. 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 was successfully obtained by using these solid-state NMR probe.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-25**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:04, 좌장: 하지원

Construction of diverse home-built solid-state NMR probes for specific purposes

정지호 김지선 김용애*

한국외국어대학교 화학과

The solid-state NMR has been used to investigate insoluble materials in advanced industrial site. It could be applied to a broad range of organic/inorganic nano-materials including polymers and bio-solids including pharmaceutical drugs and membrane proteins. Solid-state NMR spectroscopy is very valuable to study the structure and dynamics of membrane proteins even though most biological samples on lipid bilayers have high dielectric property due to containing large amounts of lipids, water and salts. We try to make the specific probe with high efficiency and durability for biological samples. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore(WB) & narrow bore(NB) 1H-15N solid-state NMR probe and a home-built 800 MHz 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 batterypack samples. These two probes provide high efficiency and good RF homogeneity.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-26**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 10:06, 좌장: 하지원

[발표취소] Theoretical calculation of collision cross section for ions in nitrogen buffer gas

고태원 김준곤*

고려대학교 화학과

발 표 취 소

본 논문은 발표취소된 논문입니다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-27**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:08, 좌장: 하지원

Stability of N-glycans Found in Human Saliva using Nano LC Chip/Q-TOF MS

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For the past decades, saliva glycans hold the attention as a potential bio-signature in clinical and forensic field owing to its inherent advantages; easy access, simple storage, and non-invasive collection. Glycosylation, one of the most common PTMs, plays an important role in a wide range of biological processes. Saliva glycosylation could be altered in the physiological and pathological situations by diseases, external environment, and chemical materials. Although profiling of glycans in saliva for the discovery of potential biomarkers for inflammatory diseases and cancers has been actively performed, fundamental studies such as saliva stability and glycans variations between individuals have been rarely done. In this study, we have investigated variations of saliva N-glycans 1) between individuals (n=18), 2) by a single individual using saliva collected on different days (0, 1, 7, and 30 days), and 3) during the storage of saliva (0, 1, 2, 3, and 7 days) in room temperature. Saliva N-glycans were enzymatically released by PNGase F and then purified and enriched by PGC-SPE. Saliva N-glycans were fully characterized by nano LC chip/Q-TOF MS and MS/MS. Inter- and intra-individual and environmental variations were qualitatively and quantitatively examined through glycan compositions and abundances. This study may help design the experiments and evaluate the saliva glycan candidates for biomarker study.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-28**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:10, 좌장: 하지원

Characterization of Glycan Signatures of Human Saliva using Nano LC Chip/Q-TOF MS

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In recent years, saliva has been received attention in forensic field. Saliva encountered at crime scene is one of the most significant evidence and thus, the identification and differentiation of saliva from other human and non-human fluids is an essential prerequisite prior to further crime investigation. However, conventional methods including enzymatic and chemical amylase test to determine saliva have lack of specificity due to cross-reactivity with other fluids. Glycoproteins are the major components of human saliva. Therefore, glycosylation in saliva can be used as a potential candidate of signature of human saliva. Herein, we have explored the possibility of nano-LC/MS-based glycomic approach to identify and differentiate bio-signature between human saliva and other fluids. Briefly, N-glycans in human saliva (7 males and 11 females) were enzymatically released and enriched by PGC-SPE. Human saliva N-glycans were profiled by nano LC-PGC chip/Q-TOF MS and –MS/MS. Saliva N-glycans displayed a heterogeneous mixture of neutral and acidic components and the most of them were decorated with fucose (> 50%). Interestingly, highly fucosylated glycans containing from tetra to octa fucose ($Hex_{5-7}HexNAc_{4-6}Fuc_{4-8}$) were observed in high abundance in human saliva. To explore human saliva-specific glycans, human saliva was compared with other fluids such as human serum, human milk, and animal saliva (rat and bovine) we conclusively determined that highly fucosylated N-glycans were saliva-specific molecules found in only human saliva. Of them tetra fucosylated bi-antennary ($Hex_5HexNAc_4Fuc_4$) and tri-antennary ($Hex_6HexNAc_5Fuc_4$) glycans were present in all human saliva.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-29**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:12, 좌장: 하지원

High-throughput Screening of Native Glycans on Therapeutic Glycoproteins using Liquid Handling System

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Glycosylation of biotherapeutics is critically associated with the stability, biological activity, half-life, and safety of drug. The glycosylation could be changed by production environment such as host cell system and culture conditions. Therefore, monitoring the glycosylation at each stage of manufacture process is a suitable approach to assess production quality for drugs. Automative high-throughput tools are currently developed and innovated to treat a large number of samples in a short time span and get high quality data by minimization of hands-on time. Here we have developed the automated analytical platform to enrich and fractionate native glycans using liquid handling system combined with 96-well microplate for a high-throughput manner. Human IgG used as a motif of therapeutic mAbs, a well known glycoprotein, was chosen to develop sample preparation procedure. Overall processes including protein denaturation by heating block, N-glycan release by PNGase F, and glycan purification and enrichment by solid phase extraction have been streamlined and optimized. Glycans were profiled by nanoLC chip/Q-TOF MS. We found total 24 glycans consisting of complex/hybrid type N-glycans w/wo sialic acid residues in both automated and manual treatment. The CVs of normalized peak intensities of top 10 N-glycans were less than 8.2 %, which indicates high comparability between two methods. Moreover, we validated the quantitative reproducibility for 5 different well positions in the 96-well plate. Two independent replicates experiments were performed per day. The Pearson correlation coefficient R between all samples was determined to be above 0.9. Glycan preparation using the automated platform showed to be rapid, reproducible, and reliable and it can be applied for real therapeutic glycoproteins.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-30**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:14, 좌장: 하지원

Assessing Biosimilarity of Therapeutic Glycoprotein using Intact Glycopeptide

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Therapeutic glycoprotein exhibits structural heterogeneity and complexity due to co-occurred glycans on a protein. Drug’s glycosylation has enormous effect on biological activity, immunogeneicity, and serum half-life. Therefore, glycomic characterization is of great importance to prove drug’s quality. With the increase of biosimilars, analytical tools for glycan profiling have been developed to evaluate the compatibility with the reference drug in efficacy and safety. Here, we present an analytical strategy to determine glycosylation similarity of therapeutic glycoproteins using intact glycopeptide. As a proof of concept, we selected recombinant erythropoietins (rhEPOs) having multiple glycosylation sites and glycan variants. The rhEPO was treated using specific protease, trypsin, to obtain glycopeptides having sugar moieties with peptide tag. We determined two intact glycopeptides of rhEPO in LC/MS analysis. One is major glycopeptide containing two N-glycosylation sites (83Asn and 88Asn), which indicates a distinctive glycosylation pattern with different O-acetylation on NeuAc. The other glycopeptide having three N-glycosylation sites (38Asn, 30Asn, and 25Asn) was also identified by glycan correlation. Using intact glycopeptide analysis, we could rapidly screen the glycoform distribution of rhEPOs for assessing biosimilarity.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-31**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:16, 좌장: 하지원

Optical Properties of Urchin-Shaped Gold Nanoparticles under Single Particle Spectroscopy

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울산대학교 화학과

Plasmonic gold nanoparticles have received much attention because of their unique size- and shape-dependent optical properties induced by localized surface plasmon resonance (LSPR) effect. In this study, we investigated the optical properties of urchin-shaped gold nanoparticles with sharp and short tips on their surface under single particle microscopy and spectroscopy. We employed scattering-based dark-field (DF) and differential interference contrast (DIC) microscopy to elucidate the optical properties of gold nanourchins (AuNUs) at the single particle level. First, we found that the LSPR peak is redshifted for single AuNUs with sharp spikes on their surface in comparison to spherical gold nanoparticles with same size. Second, we obtained the defocused images of single AuNUs under DF microscopy, which provided three-dimensional (3D) spatial scattering field distributions. Last, we found polarization-dependent DIC images and intensities of single AuNUs under interference-based DIC microscopy, which was not observed for gold nanospheres without sharp tips. Therefore, the results allow us to have a better understanding of the optical properties of single AuNUs with the spiked surface.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-32**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:18, 좌장: 하지원

Plasmon-enhanced photoluminescence immunoassay for Influenza virus sensing by using gold nanoparticle decorated carbon nanotube

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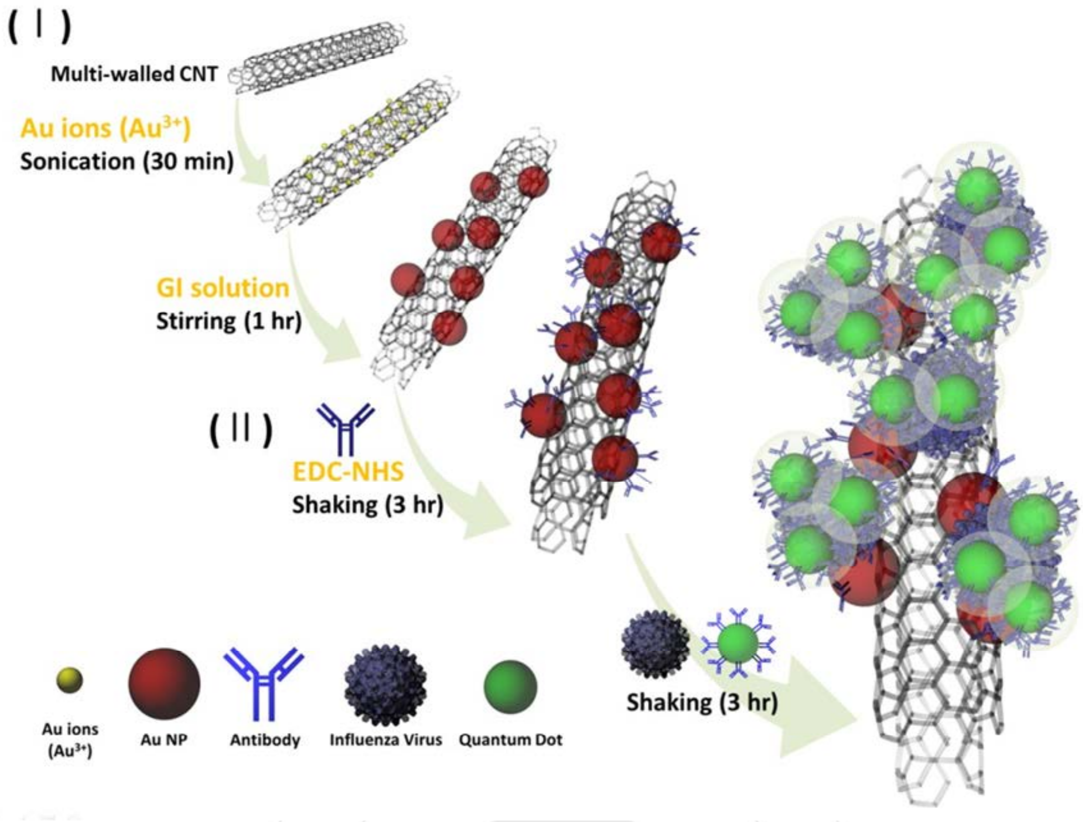
A plasmon-assisted fluoro-immunoassay (PAFI) was developed for the detection of the influenza virus by using Au nanoparticle (Au NP)-decorated carbon nanotubes (AuCNTs) that were synthesized using phytochemical composites at room temperature in deionized water. Specific antibodies (Abs) against the influenza virus were conjugated onto the surface of AuCNTs and cadmium telluride quantum dots (QDs), which had a photoluminescence intensity that varied as a function of virus concentration and a detection limit of 0.1 pg/mL for all three types of influenza viruses examined. The clinically isolated influenza viruses (A/Yokohama/110/2009 (H3N2)) were detected in the range of 50–10,000 PFU/mL, with a detection limit of 50 PFU/mL. From a series of proof-of-concept and clinical experiments, the developed PAFI biosensing system provided robust signal production and enhancement, as well as an excellent selectivity and sensitivity for influenza viruses. This nanoparticle-based technique could be potentially developed as an efficient detection platform for the influenza virus.


(Ⅰ)
Multi-walled CNT
Au ions (Au^{3+})
Sonication (30 min)
GI solution
Stirring (1 hr)
(Ⅱ)
EDC-NHS
Shaking (3 hr)
Shaking (3 hr)
Au ions (Au^{3+})
Au NP
Antibody
Influenza Virus
Quantum Dot

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-33**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 하지원

A Sandwich-type HIV-1 p24 immunoassay using ICP-MS with metal-doped nanoparticles

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A virus is a type of non-cellular infectious agent that replicates inside the host cells of other organisms. Human Immunodeficiency Virus (HIV) causes acquired immunodeficiency syndrome (AIDS) and HIV-1 p24, a component of the HIV particle capsid, is an antigen detected in infected patients' blood. For detection of HIV-1 p24, the sandwich-type conjugates employing metal-doped magnetic nanoparticles (MNPs) and metal/dye-doped silica nanoparticles (SNPs) were produced by immunoreaction and the concentration of the target was determined by ICP-MS in this work. For this, both Cs-doped Fe_3O_4 MNPs and Gd/RhBITC-doped SNPs for target extraction and tagging as a probe, respectively, were synthesized and immobilized with the antibodies of HIV-1 p24. Feasibility of quantification was shown from the calibration curve plotted the intensity ratio of Gd/Cs vs. the concentration of target. For future work, this method will be applied to real samples and multiplex detection of other viruses.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-34**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:22, 좌장: 하지원

Microwave-assisted week acid hydrolysis of proteins using hydrochloric acid generating serial detachment of amino acids

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충남대학교 화학과

Microwave-assisted week acid hydrolysis of proteins has been developed as an alternative approach for protein sequence analysis. Microwave-assisted weak acid hydrolysis of proteins can be performed with a small amount weak acid (e.g. 2%) such as formic acid, acetic acid or phosphoric acid in a microwave oven for an hour incubation. Weak acid hydrolysis cleaves exclusively C-terminal of aspartic acid. This method is simpler and faster than using a protease such as trypsin. It was reported that 3 M HCl hydrolyzed a protein into polypeptide ladders with varying sizes of up to molecular mass of the protein. Here we tried to truncate N-terminal of aspartic acid with small amount of hydrochloric acid for microwave-assisted acid hydrolysis after microwave-assisted week acid hydrolysis of myoglobin. The 0.5 ~ 1% HCl hydrolysis of C-terminal truncated myoglobin peptides provided major peptides cleaved selectively at the N-terminal of aspartic acids. The cleaved peptides was identified by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry, where the peptides cleaved with the N-terminal of aspartic acid were observed as major peaks while the peptides with the C-terminal cleavage of aspartic acid were observed as minor peaks.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-35**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 10:24, 좌장: 하지원

Auto-flame synthesis of $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ as cathode materials for Li-ion battery

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울산대학교 화학과

A simple, rapid, and efficient flame synthesis method was developed cathode materials for Li-ion batteries. Therefore, the combustion of the metal nitrate precursors with flame was used to complete synthesis of $LiNi_{0.95-x}Co_xTi_{0.05}O_2$. The complete procedure to achieve the $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ precursor powder was taken under 1 hr. X-ray diffraction (XRD) patterns confirm the formation of single phase of the $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ at 800℃ for 12hr. SEM and TEM analyses show the presence of ultrafine nature of the particles. The fabricated materials show the discharge specific capacity of 159 mAh g^{-1} and 137 mAh g^{-1} at 0.1 C-rate for the initial cycle for the $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ of $x = 0.25$ and 0.30, respectively. The results indicate that $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ synthesized with environmental friendly route shows a promising electrochemical activity.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-36**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:26, 좌장: 하지원

Excellent electrochemical performance and wide operating voltage of phosphate-borate hybrid cathode material for Li-ion battery

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울산대학교 화학과

Olivine $LiMPO_4$ (M=Fe, Mn, Co, Ni, etc.) based cathode materials for lithium ion battery widely investigated for electric vehicles and electronic device due to low cost, safety and structural stability. This work reports for the first time lithium iron phosphate and lithium iron borate as a hybrid cathode material. The material has been synthesized without using external carbon source to improve specific discharge capacity with wide operating voltage range. $LiFe(PO_4)_{0.5}(BO_3)_{0.5}$ exhibits a remarkably high specific discharge capacity near the theoretical capacity (97.3%) of 189.8 mAh g^{-1} at 0.1 C. X-ray diffraction and NMR spectroscopy of the pristine material revealed mixed phase of olivine and vonsenite structures. The electrochemical performance of the $LiFe(PO_4)_{0.5}(BO_3)_{0.5}$ showed also polymorphism with two different structured materials. The LFBP cathode material can meet the requirements for high power applications, such as electric vehicles and energy storage for smart grids in the near future.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-37**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:28, 좌장: 하지원

Detection and counting of red blood cells via electrochemical collision event on an Ultramicroelectrode

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숙명여자대학교 화학과 [1]전북대학교 화학교육과

Information about blood tests is very necessary for diagnosing and detecting blood disorders. Here, we have developed the electrochemical detection of red blood cells (RBCs) using single particle collision events. The staircase current decrease was caused by collision, and gave quantitative information about the size, and concentration of RBCs. The signals obtained by chronoamperometry (CA) measurement during a collision of RBCs with ultramicroelectrode (UME) at the different of RBCs concentration showed high sensitivity and will be essential in the future.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-38**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 하지원

Detection of water/oil nanoemulsion droplet using electrochemical collisions on an Ultramicroelectrode

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숙명여자대학교 화학과 [1]전북대학교 화학교육과

Herein, for the first time, research on water/oil emulsion droplet by electrochemical analysis has been reported. By the use of blocking of the single emulsion droplet, water/1,2-dichloroethane emulsion droplets collided with an ultramicroelectrode (UME) leading to the “stair-case” current decrease. Each “stair-case” current decrease corresponds to the emulsion droplet collision on UME surface. The experimental collision frequency is proportional to the concentration of emulsion droplet. In addition, each water droplet size was estimated from the magnitude of the “stair-case” current decrease with simulation data. Results obtained from the collision signals provide information about the single droplet size (nano- to micro-) and a pM concentration of the water emulsion in organic continuous phase.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-39**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:32, 좌장: 하지원

Using Electromembrane Extraction for Determination of NSAIDs by HPLC-UV

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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 four Non-steroidal anti-inflammatory drugs(NSAIDs) in human urine samples. The parameters such as pH of acceptor, stirring speed, voltage, support liquid membrane(SLM), and extraction time were optimized. Simultaneous chromatographic separation of four 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 30:70 and after 5minutes, compositon is changed to 15:85, finally, changed to 5:95 after 5minutes. After the extraction, 5 μℓ of extract was directly injected into the HPLC-UV system.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-40**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:34, 좌장: 하지원

Feasibility of a compact low-cost laser-induced breakdown spectroscopy device for quantitative analysis of metallic elements in edible salt products

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목포대학교 화학과

We investigated feasibility of a compact low-cost laser-induced breakdown spectroscopy (LIBS) device for quantitative analysis of Ca and Mg in edible salts. By using a compact low-power diode-pumped solid-state (DPSS) laser and a miniature non-gateable charge-coupled device (CCD) spectrometer, the LIBS spectrometer could be significantly simplified. The standard materials were prepared using mixtures of NaCl, $MgSO_4$, and $CaCO_3$ in forms of solid pellets. The DPSS laser beam (270 microjoule/pulse) was focused on the pellet surface through an objective lens. Optical emission from the laser-induced plasma was collected and sent to the non-gateable miniature CCD spectrometer. For each concentration of Ca or Mg, the averaged emission line intensity from the measurements for multiple pellets provided the improved analysis precision in comparison with that obtained from multiple line scans for a single pellet. This indicates that the chemical composition was homogeneous enough and however the measurement condition was not consistent among the multiple line scans within the same pellet. The fluctuation could be averaged out by taking data from multiple pellets. We applied this device and analysis methology to real salt products and discussed its feasibility as a portable in-situ analysis device for salt products.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-41**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:36, 좌장: 하지원

Fabrication and Application of the Microfluidic Devices Designed to Simulate HET-CAM Test

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공주대학교 화학과

In this presentation, we will describe the development and application of a simple microfluidic device for in vitro irritation tests of cosmetics. The device was fabricated with a three-compartment diffusion system to mimic the HET-CAM system. HUVEC (Human Umbilical Vein Endothelial Cells) was cultured in the three compartments and the tested substances were injected to the reservoir and diffused through the tiny microfluidic channels. The viability of cells in each compartment was monitored by an optical microscope. The IS (irritation score) values were evaluated based on the viability of cells as a function of time when the cells were exposed to the tested substances. Three kinds of cosmetic materials were tested with microfluidic systems, and the results were compared with those of the HET-CAM test to validate the in vitro irritation test system.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL1.O-42**

발표분야: Oral Presentation of Young Analytical Chemists Ⅰ

발표종류: 구두발표, 발표일시: 목 10:38, 좌장: 하지원

Electrochemical Detection of Hydrazine Using Poly(dopamine)-Modified Electrodes

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We have developed a simple and selective method for the electrochemical detection of hydrazine (HZ) using poly(dopamine) (pDA)-modified indium tin oxide (ITO) electrodes. Modification with pDA was easily achieved by submerging the ITO electrode in a DA solution for 30 min. The electrocatalytic oxidation of HZ on the pDA-modified ITO electrode was measured by cyclic voltammetry. In buffer solution, the concentration range for linear HZ detection was 100 µM–10 mM, and the detection limit was 1 µM. The proposed method was finally used to determine HZ in tap water to simulate the analysis of real samples. This method showed good recovery (94%–115%) and was not affected by the other species present in the tap water samples.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-43**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 하지원

Determination of the Inorganic Arsenic with Solid Phase Extraction and LIBS

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The toxicity, bioactivity and mobility of arsenic are dependent on the chemical forms or species in which it exists. It is well known that the inorganic arsenic is more toxic than the organic arsenic. The ICP-MS coupled with chromatographic techniques has been used to perform the qualitative and quantitative determination of the arsenic species in various samples. However, it has been difficult to conduct a overall analysis due to matrix effects and took a long time to separate the arsenic species in various samples with the complex matrix. In this study, the solid phase extraction(SPE) membrane was used to separate inorganic arsenics, and those were detected by laser induced breakdown spectroscopy (LIBS). The samples were prepared using a buffer solution with phosphate buffer saline (pH 7.4) to separate arsenic species. The recovery efficiency of As(Ⅴ) by LIBS was 106.7 %. The separated As(Ⅲ) was identified by IC-ICP-MS. From the results, it was confirmed that inorganic arsenic species could be separated and detected using SPE membrane and LIBS.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL1.O-44**
발표분야: Oral Presentation of Young Analytical Chemists Ⅰ
발표종류: 구두발표, 발표일시: 목 10:42, 좌장: 하지원

Synthesis and characterization of graphene-enfolded mesoporous TiO2 microsphere as anode material for Li secondary batteries

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In this study, graphene-bonded and enfolded mesoporous anatase TiO2 microsphere (GMTMs) composites have been synthesized without using any cross-linking reagent, by using graphene oxide (GO) and titanium glycolate microsphere (TGMs) as a precursor. Monodispersed and uniform mesoporous TiO2 microspheres with a tunable diameter were fabricated by the facile aqueous route, nano-particle microspheres are interconnected 10-20 nm in size. TGMs diameter tuned from 100 to 800 nm with consistent size and morphology by changing the amount of water. GO sheets were enfolded on TGMs by covalent bond after a subsequent refluxing. Crystallization of TiO2 and reduction of GOMTMs was dramatically marked up by hydrothermal and calcination in an Ar atmosphere. The physicochemical properties were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Field emission scanning electron microscopy (FE-SEM), Transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy. Surface areas were also measured by BET method. The electrochemical performance of TGMs composites as anode for Li secondary batteries were investigated by cyclic voltammetry, galvanostatic charge/discharge, and impedance spectroscopy. TGMs composite with higher surface area showed better electrochemical performance in charge capacity and cycle ability. AcknowledgementsThis research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO.2015035858)

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-1**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:00, 좌장: 김병권

Evaluation of Laser-Induced Breakdown Spectroscopy as a simple method for identifying geographical origins of agricultural products

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한양대학교 화학과

Fast identification of geographical origins of agricultural products becomes more demanding recently. For this purpose, Raman and near-infrared (NIR) spectroscopy have been widely employed since the corresponding measurements are fast and non-destructive with minimal or no sample pretreatments. These spectroscopic methods provides molecular structural information of sample components for the identification; while, the difference in atomic composition in samples is alternatively valuable in many cases. Therefore, laser-induced breakdown spectroscopy (LIBS), which can provide information on almost all elements, has gained an attention. LIBS-based measurement is also fast as nearly non-destructive as comparable with Raman and NIR spectroscopy. Here, we have utilized LIBS for the identification of geographical origin of milk vetch root. The pellets made from domestic and imported milk vetch root samples were measured and the acquired LIBS spectra were used for the discrimination using several chemometric methods. For the collection of representative spectra, LIBS spectra acquired at different spots on each pellet were averaged. The resulting discrimination accuracy was evaluated in conjunction with the difference in the composition of elements.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-2**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:10, 좌장: 김병권

Setting up Overhauser Dynamic Nuclear Polarization Nuclear Magnetic Resonance Systems

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낮은 에너지를 사용하는 Nuclear Magnetic Resonance(NMR) 기법은 분자 구조와 운동을 비파괴적으로 관찰할 수 있으며, 비결정 시료 또한 분석이 가능하고, 관찰하고자하는 핵종을 선택 할 수 있어 선택성이 높다는 등의 장점을 가지고 있다. 하지만 NMR 은 낮은 에너지의 주파수를 사용하기 때문에 낮은 감도로 핵스핀 신호를 얻는다는 단점을 가지고 있다. 이러한 단점을 보완하기 위해서 본 연구에서는 전자스핀과 핵스핀의 상호작용을 통해 NMR 신호를 수십에서 수백 배까지 증폭시키는 장비인 Overhauser Dynamic Nuclear Polarization(ODNP) NMR 시스템을 Electron Paramagnetic Resonance(EPR) 장비에 NMR 부품(RF Pulse 모듈, NMR tuning box, ODNP NMR probe 등)을 결합하는 방법을 사용하여 ODNP NMR 을 구축하고자 한다. ODNP NMR 에서는 스핀표지자의 전자스핀 중심 반경 약 1 nm 내의 핵 스핀들과 주로 상호작용을 하여 NMR 신호가 증폭된다. 따라서 스핀표지자를 이용하여 측정하고자 하는 국소 부위를 지정할 수 있으며 고분자 물질내의 물의 확산속도, 용매 따른 단백질과 물의 결합 변화 등을 측정하는데 활용 할 수 있다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-3**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:12, 좌장: 김병권

Proton Nuclear Magnetic Resonance Spectroscopic Investigation of Inner Channel-Surface Change of Nafion upon Chemical Degradation

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고분자 전해질 막은 연료전지의 핵심 구성 소재로 많이 사용하는데 장시간의 연료전지 운영에 의하여 열화가 일어날 수 있다. 대표적인 고분자 전해질 막인 Nafion(나피온)의 경우, 수 많은 연구 결과에서 열화 산물로 나피온의 SO_3H 가 떨어지고 OH 로 대체되어 생긴 CF_2OH 를 주로 보여주었다. 하지만, 최근 문헌에서는 CF_2H 도 열적 열화의 산물임을 새롭게 제시하였다.이를 바탕으로 본 연구에서는 화학적 열화에서도 CF_2H 가 생성 되는지와 이 때, 친수성 채널 안에 있는 물이 받는 영향을 보고자 하였다. Fenton 반응을 1, 3, 6 시간 동안 진행하여 준비한 모든 나피온 시료에서 ~6.9ppm 에 CF_2H 의 신호가 나오는 것을 ^1H magic-angle spinning nuclear magnetic resonance spectroscopy 를 이용하여 확인하였다. 또한 Fenton 반응이 진행됨에 따라 나피온이 함유하는 물의 함량 (λ')은 감소하여 Fenton 반응을 6 시간 시킨 시료의 경우, λ'이 0 으로까지 감소하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-4**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:14, 좌장: 김병권

Investigation of Electrochemical Reactions in Direct 2-Propanol Fuel Cells(DPFCs) by ^{13}C Nuclear Magnetic Resonance Spectroscopy

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알코올 중 propanol 은 methanol, ethanol 에 비해 물과 이산화탄소만 생성하는 완전한 산화를 한다면 전자를 생산할 수 있는 에너지 발생 밀도가 크다는 이점을 가진다. 하지만 실제로는 propanol 연료전지의 경우 대부분 불완전 산화가 일어나고, 전극의 피독 현상이 일어나며, 연료가 양극에서 음극으로 넘어가는 크로스오버 현상이 일어나는 문제가 있다. 따라서 본 연구에서는 다양한 조건에서 2-propanol 연료전지를 운영하며 전기화학적 장비를 통해 얻은 정보와 양극과 음극 배출액의 ^{13}C Nuclear Magnetic Resonance (NMR) 스펙트럼들로부터 생성물의 규명 및 정량 분석을 수행하였다. 이를 통하여 연료극과 공기극 배출액의 화학적 조성이 연료전지의 성능에 따라 어떻게 변하는지 추적하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-5**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:16, 좌장: 김병권

SERS-based immunoassay for the simultaneous detection of two prostate-specific antigens in clinical serum

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Numerous studies showed that the clinical accuracy of the prostate-specific antigen (PSA) determination can be improved by measuring the ratio of either free PSA (f-PSA) or complex PSA (c-PSA) relation to total PSA (t-PSA). Enzyme-linked immunosorbent assay (ELISA) and photoluminescence bioassays have been widely used for the quantitative analysis of PSA in clinical laboratory. However, those techniques have some technical drawbacks such as poor signal-to-noise ratio, limit of detection and simultaneous multiplex detection capability. Thus, scientists and medical doctors are still concerned about the ways to improve the PSA immunoassay test for the precise diagnosis of prostate cancer. In this work, a novel SERS-based immunoassay platform, using gold nanoparticles and magnetic beads, has been developed for the simultaneous detection of f-PSA and c-PSA. Here, XRITC- and MGITC-labelled gold nanoparticles have been used as SERS nanotags for the dual PSA marker assay. On the other hand, magnetic beads have been used as supporting substrates for the high density loading of immunocomplexes. Using this simultaneous assay platform, the SERS-based assay data for 30 clinical samples were obtained and compared with those measured by the chemiluminescence instrument installed in clinical laboratory. Compare with a parallel assay, the simultaneous assay shows more precise result and also has better reproducibility. This SERS-based technique provides a new insight for the fast and accurate diagnosis of prostate cancer.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-6**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:18, 좌장: 김병권

SERS-based immunosensor for the highly sensitive detection of mycotoxin using three-dimensional nano-pillar array chips

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Mycotoxins such as ochratoxin A, aflatoxin B1, fumonisin and others are well-known dangerous food contaminants that usually occur in trace amounts from nanograms to micrograms per gram of food. Due to their teratogenic and carcinogenic properties, mycotoxins present a serious hazard to human and animal health. The conventional detection methods such as high-performance liquid chromatography, mass spectroscopy and ELISA are extensively used for their quantitative analysis but they are rather expensive or time consuming; therefore, a new detection technique is still needed for the rapid and sensitive detection of Mycotoxins. For this purpose, we designed a novel SERS-based immunosensor for mycotoxin detection by combining a three-dimensional (3D) nano-pillar array chip with a surface-enhanced Raman scattering (SERS) detection technique. Upon target mycotoxins and mycotoxins antibody introduction, a competitive-type immunoreaction was implemented between the target and the immobilized mycotoxins-BSA on the 3D nano-pillar array chip. After this reaction, secondary antibodies conjugated on SERS nanotags were captured on the 3D nano-pillar array chip surface, forming a confined 3D plasmonic field, leading to the enhanced electromagnetic field on the 3D pillar surface. This work is expected to be a potentially useful tool for the rapid and sensitive detection of various mycotoxins.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-7**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:20, 좌장: 김병권

Various analytical methods for the determination of the arsenic species in rice

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The qualitative and quantitative determination of the total arsenic as well as the arsenic species in rice has been very important. However, it has been troublesome due to the matrix interference. In this study, the various analytical methods including the internal standard method and standard addition method have been investigated for the determination of arsenic species in rice. The four different arsenic species in rice have been separated by ion chromatograph, then detected by ICP-MS (inductively coupled plasma mass spectrometry). In addition, the various extraction methods by the nitric acid and the malonic acid have been also investigated. The quality control for rice was done with certified reference material (NIST 1568b CRM). The malonic acid extraction method showed 83 % recovery for the total arsenic, but only 58% recovery for inorganic arsenic. The nitric acid extraction method showed the overestimated results of 114 % recovery to total arsenic. We have used the nitric acid extraction method using arsenobetain as internal standard to improve the accuracy. Thus, we have acquired 96% and 66% recoveries for the total arsenic and inorganic arsenic, respectively. In addition, we have used the standard addition method to reduce the matrix interference. We have acquired 127 % and 111 % recoveries for the total arsenic and inorganic arsenic, respectively.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-8**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:22, 좌장: 김병권

Amperometric antibiotics sensor using liquid/gel interfaces

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본 포스터에서는 서로 혼합되지 않는 두 전해질 (수용성 액체/유기성 젤) 계면에서 전하를 띈 항생제가 선택적으로 이동하는 반응에 따라 변화하는 전류값을 측정하는데 기반을 둔 이온 선택적 전류법 센서 개발에 관한 연구를 나타냈다. 수용성 액체와 유기성 젤 사이에 계면을 형성하고 수용액 액체의 pH 가 변할 때 항생제 이온의 전하도 달라진다. 이를 검출하기 위해 특정 pH 에서 전압을 걸어주게 되면 항생제 이온의 농도에 따라 계면에서 전이하는 정도의 차이에 따라 전류가 어떻게 변화하는 지를 순환전압전류법(cyclic voltammetry)과 시차 펄스 벗김 전위법(different pulse stripping voltammetry)으로 정량적으로 분석하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-9**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:24, 좌장: 김병권

알칼라인 이온성 액체의 합성

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본 연구실에서는 보다 쉬운 방법으로 여러 가지 성질(열에 잘 견디며, 낮은 증기압, 높은 이온전도도, 환경 친화적)을 지닌 점성질의 이온성 액체를 개발하고 있다. 이 이온성 액체는 실온 이온성 액체라고도 불리우며 유기합성, 촉매, 연료 전지 외에 여러 분야에서 다양하게 이용되고 있다. 유(무)기 양이온과 유(무)기 음이온을 여러가지 (극성, 무극성)용매를 이용하며, 합성물을 pH, 전기전도도와 정성 분석을 통하여 합성유무를 확인해 보았다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-10**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:26, 좌장: 김병권

액체 / 액체 계면에서의 Tetracycline 전달 및 감지 응용의 Voltammetric 연구

LIU XIAOYUN 이혜진*

경북대학교 화학과

두 가지의 혼화되지 않는 전해질 용액 (ITIES) 사이의 분극화 된 계면을 통한 이온 전달 과정은 다양한 유형의 이온 선택성 감지 플랫폼을 만드는데 이용되어왔다. ITIES 를 통한 이온 전달 반응은 약물 분자의 친 유성을 이해하기위한 강력한 도구로 사용될 수 있다. 다양한 금속 이온, 음이온 및 전반의 전하를 띄는 약물 분자를 포함한 광범위한 이온 종의 연구가 액체 / 액체 계면를 통해 이루어졌다. ITIES 에서 다양한 약물 종의 전이 반응에 대한 많은 전기 화학적 연구 결과가 보고되었지만 항생제 또는 기타 질병 치료제의 정량 분석을위한 감지 플랫폼으로 ITIES 의 설계를 보여주는 보고서는 거의 없다 .

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-11**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:28, 좌장: 김병권

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

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Graphene has been reported as an excellent lubricant additive for reducing adhesion and friction when coated on various surfaces as an atomically thin material with low surface energy. We have developed graphene oxide (GO) grafted with long alkyl chains to improve dispersion in oil-base lubricant as largely enhanced lipophilicity. Alkyl functionalized GO is synthesized by reacting NH2-GO with butylchloride, octylchloride in ethanol under reflux, then 1.0x10-3 wt% of alkyl functionalized GO are added into the base oil (PAG oil) and ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene are investigated by Fourier transform infrared (FT-IR), 13C solid-state nuclear magnetic resonance (13C NMR), X-ray diffraction (XRD), and scanning electron microscope (SEM). The tribological tests are performed with a tribometer and the test mode is ball-on-disk. The van der Waals interaction between the octyl chains grafted on GO and the alkyl chains of base oil provided long-term dispersion stability so that the octyl functionalized GO showed better dispersion than butyl functionalized GO. The octyl functionalized GO also decreased both friction and wear considerably under the rubbing contacts between ball and disk. Acknowledgements: This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2015035858).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-12**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:30, 좌장: 김병권

Synthesis and characteristics of reduced graphene oxide/mesoporous silica composites as anode materials for lithium secondary batteries

손빛나 현유라 배재영 박희구[1] 이창섭*

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The reduced graphene oxide/mesoporous silica composites (rGO/m-S) as a high performance anode for lithium secondary batteries have been synthesized. The rGO/m-S composites with different mass ratios are dissolved in distilled water and coated on a Nickel foam via a simple dip-coating method. Nickel foam is used as a current collector and template for the electrode fabrication. The physicochemical characteristics of the rGO/m-S composites were analyzed by scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy, N_2-sorption and X-ray photoelectron spectroscopy (XPS). A three-electrode cell, as a half cell, was assembled by using rGO/m-S composites as the anode active materials of lithium secondary batteries in a glove box filled with Ar gas. The prepared rGO/m-S materials were used as the working electrode. Lithium was used as the counter and reference electrodes. A glass fiber separator was used as the separator membrane. 1 M $LiClO_4$ was used as the electrolyte and dissolved in a 1:1 volume mixture of ethylene carbonate:propylene carbonate 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. Li secondary batteries prepared with mixed rGO/m-S composite showed better electrochemical performance than the case of multilayered rGO/m-S composite. Acknowledgements This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2015035858).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-13**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:32, 좌장: 김병권

Amperometric detection for antibiotic molecules using carbon modified electrode

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An electrochemical biosensor was developed for detection of antibiotic molecules using sandwich assay format involving two bioreceptors for the target molecules. This sandwich format was examined on carbon screen printed carbon electrode (SPCE) surface. The binding of antibiotic molecule to both bioreceptors were analyzed by cyclic voltammetry and different pulse voltammetry with different target concentrations. Quantitative analysis of the target concentrations is also reported.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-14**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:34, 좌장: 김병권

Detection of antibiotic molecules using metallic nanoparticles modified screen printed carbon electrode

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Antibiotics are used to treat bacterial infection, while the abuse can cause a lot of side effects. An amperometric sensor fabricated on gold nanoparticle(NPs) modified screen printed carbon electrodes(SPCEs) is demonstrated for the detection of antibiotic molecules. The developed sensor's electrochemical characteristics and performance were thoroughly investigated using cyclic voltammetry and differential pluse voltammetry.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-15**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:36, 좌장: 김병권

The synthesis of polydopamine to composite with multi-walled carbon nanotubes for modification of the glucose dehydrogenase into the electrode

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Polydopamine (PDA) was used as a biocompatible polymer that has been used in various fields ranging from material aspects, drug delivery, and bio-sensing. We has used as a biosensor multi-walled carbon nanotubes (MWCNTs) coated with PDA to improve sensitivity and reproducibility. MWCNTs was easily coated with PDA at room temperature by mildly stirring. The PDA immobilized MWCNTs (PDA/MWCNTs) solution was loaded onto indium-tin oxide (ITO) electrode. And after using mixed solution with 1-ethyl-3-(3-dimethyl aminopropyl) carbodiimide (EDC) and N-hydroxysuccinimide (NHS) to activate PDA/MWCNTs/ITO electrode, GDH was modified to the electrode. The morphological and thermal characterization of GDH-PDA/MWCNTs/ITO electrode was measured by field emission scanning electron microscope (FE-SEM) and thermogravimetric analyzer (TGA), respectively. And the electrical signal was checked by cyclic voltammetry (CV). Also, GDH-PDA/MWCNTs/ITO electrode wasn't affected by interferences such as ascorbic acid (AA) and uric acid (UA). Therefore, our study has shown that possibility for applying as a biosensor.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-16**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:38, 좌장: 김병권

Theinterface correlation between multi-walled carbon nanotubessize with hydrophilic polymer and dispersion

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Abstract: The hydrophilic dispersion of multi-walled carbon nanotubes (MWCNTs) have been studied causing its biocompatible properties for applying as biomaterials. In this study, the interface correlation between dispersion and multi-walled carbon nanotubes which has another size were investigated. The MWCNTs was treated by ultrasonic with hydrochloric acid (HCl) to control the size of that. The different size of MWCNTs were composited with poly(acrylamide)-poly(vinylpyridine) (PAA-PVP) hydrophilic polymer. The physicochemical characterization of PAA-PVP composites with MWCNTs were examined by particle size analyzer (PSA), X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM).And electrochemical impedance was measured by potentiostat. Finally, the zeta potential was used for interface correlation between MWCNTs size and dispersion. The results showed that the size of MWCNT for dispersion is very important.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-17**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:40, 좌장: 김병권

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

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We have performed a study of a silica/carbon nanocoils (SiO_2-CNC) nanocomposite as a potentially high performance anode for rechargeable lithium secondary batteries. Carbon nanocoils were grown via chemical vapor deposition (CVD) method. Acetylene (C_2H_2) and Sulfur hexafluoride (SF_6) were flowed into the quartz reactor of a tubular furnace heated to 550 ℃ at 100 torr and maintained for 60 min to synthesize CNCs. CNCs were then put into the Tetraethyl orthosilicate (TEOS) to synthesize SiO_2-CNCs composite. The electrochemical characteristics of SiO_2-CNCs composites as an anode of Li secondary batteries were investigated using three-electrode cell. The SiO_2-CNCs composites loaded on Ni foam were directly employed as an working electrode without binder. As the counter and reference electrode used lithium foil. 1M $LiClO_4$ was employed as electrolyte and dissolved in a mixture of propylene carbonate (PC): ethylene carbonate (EC) in a 1:1 volume ratio. Glass fiber separator was used as the separator membrane. The galvanostatic charge–discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. The morphologies, compositions and crystal quality of the prepared SiO_2-CNCs composites were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), energy X-ray diffraction (XRD), dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). As a result electrochemical performance of SiO_2-CNC was batter than existing carbon nanofibers and carbon nanocoils.AcknowledgementsThis research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2015035858)

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-18**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:42, 좌장: 김병권

Electrochemical Studies on Anti-Cancer Drug Transfer Across Water/Oil Interface

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In this study, the ion transfer mechanism of an anthracycline derived anticancer drug at a polarized interface between two immiscible electrolyte solutions (ITIES) has been investigated. The voltammetric technique has been applied to study the ionization of the drug molecule at different pH of aqueous solution and organic solution interface. Some of preliminary results were demonstrated and a potential analytical purpose for sensing application of this work was also investigated in this work.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-19**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:44, 좌장: 김병권

A SERS-based magnetic immunoassay of fraction 1 antigen for Yersinia pestis utilizing integrated droplet microfluidics

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The combination of surface-enhanced Raman scattering (SERS)-based detection technique with lab-on-a-chip platform provides an ideal mechanism for achieving rapid, sensitive and reproducible assay 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, and its application to clinical diagnostics. 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 device was designed and fabricated for a sequential immunoassay processing in an automatic manner. This device is composed of six distinct compartments including droplets generation, mixing, merging, isolation, separation, and detection. Herein, we report a novel SERS-based droplet microfluidic device for fully automatic immunoassay in the microfluidic channel. For the proof-of-concept, the device was applied to the detection of the fraction 1 antigen of plague marker which is well known as an important anti-phagocytic antigen of Yersinia pestis.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-20**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:46, 좌장: 김병권

iCCM-based isotope dilution mass spectrometry for absolute quantification of human growth hormone and brain natriuretic peptide-32 in human plasma

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Isotope dilution mass spectrometry (ID-MS) has been used as a primary method for the absolute quantitative determination. Although the conventionally absolute quantification (e.g., synthetic proteins or peptides) or stable isotope labeling methods (e.g., ICAT, mTRAQ) in quantitative proteomics have been considered as a reliable approach in shotgun proteomics, these methods have unfortunately several bottlenecks such as imperfect labeling, and time consumption of labeling for proteome samples. To improve above-mentioned problems, we applied the carbamidomethylation-based isotope labeling (iCCM) for absolute quantification of hGH and BNP-32 in human plasma in this study. To evaluate the iCCM labeling for absolute quantification, plasma sample was first labeled with iodoacetamide (IAA) as carbamidomethylation (CM), while both human growth hormone (hGH) and brain natriuretic peptide-32 (BNP-32) standards were isotopically alkylated with IAA isotope (IAA-13C2D2) as iCCM, followed by spiking those iCCM-labeled standards to plasma sample labeled with CM. The resulting plasma sample was directly performed tryptic digestion and subsequently applied to nLC-ESI-MS/MS analysis so as to obtain the absolute amounts of both hGH and BNP-32. In conclusion, iCCM-based ID-MS provides the simple, rapid, and high reproductive method for the assessment of the ratio of CM/iCCM, resulting in absolute quantification of hGH and BNP-32.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-21**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 09:48, 좌장: 김병권

Efficient use of separation space in two-dimensional liquidchromatography system for extensive and efficient proteomicanalyses

이한겨레 이상원*

고려대학교 화학과

Proteomics aims to complete profiling of the protein content and their modifications in cells, tissues, and biofluids and to quantitatively determine changes in their abundances. This information reveals cellular processes and signaling pathways and serves to identify candidate protein biomarkers and/or therapeutic targets. Therefore, analysis should be comprehensive and efficient. Here, we present a novel online two-dimensional reverse-phase/reverse-phase liquid chromatography separation platform, employing a newly developed online non-contiguous fractionating and concatenating device (NCFC fractionator). In bottom-up proteomics analyses of a complex proteome, this system provided significantly improved exploitation of the separation space of the two RPs, resulting in a considerable increase in the numbers of peptides identified compared to a conventional contiguous 2D-RP/RPLC method. The fully automated online 2D-NCFC-RP/RPLC system bypassed a number of labor-intensive manual processes (offline fractionations, poling, clean-up, drying/reconstitution, and autosampler fraction injection) required with previously described offline 2D-NCFC-RP/RPLC method, offering minimal sample loss and highly reproducible 2D-RP/RPLC experiments.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-22**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:50, 좌장: 김병권

Development of advanced proteome-to-genome mapping technologies and application to proteogenomic characterization of early onset gastric cancer

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고려대학교 화학과

Next-generation sequencing and MS-based proteomics have been increasingly adopted as powerful technologies for characterizing cancer genome and proteome. Also there have been endeavors for integrating genomic and proteomic data to achieve comprehensive understandings of cancer. To this end, sensitive, extensive, and quantitative profiling of proteome are needed. In this study, advanced proteome-to-genome mapping (P2G) technologies were developed, including standardized proteome sample preparation procedure, serial enrichment of PTMs, highly sensitive LC-MS/MS analysis platform, and improved post-experimental peptide identification tool. Developed P2G mapping technologies were applied for characterizing proteome of early onset gastric cancer. Global proteome, phosphoproteome and N-glycoproteome profiling were performed for paired tumor and adjacent normal tissues of 80 patients. Obtained proteome profiles were integrated with genomics data (e.g. exome and mRNA data), which provided additional knowledges on cancer biology that were not obtainable by genomic data only.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-23**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:52, 좌장: 김병권

Influence of sedimentation on the cellular association and endocytosis mechanisms of silver nanoparticles: Flow cytometry and ICP-MS study

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Recently, nanomaterials have attracted increasing interest and widely used in many applications, such as nanomedicine as well as consumer products. However, their accumulation in the environment raises concerns on the potential hazards of nanomaterials on biological and environmental systems.1 Silver nanoparticles (Ag NPs) are widely used as antimicrobial agents, laundry detergents, wall paint and clothing such as underwear and socks.2 Notwithstanding the increasing use of Ag NPs in consumer products and potential risk of human exposure, there is no quantitative understanding on their cellular association mechanism and resultant toxicity .3 To better understand these phenomena, it is prerequisite to develop measurement method and perform quantitative analysis of intracellular Ag NPs.4The purpose of this study is to investigate the influence of nanoparticle sedimentation on their cellular association and related endocytosis mechanism, when A549 cells were exposed to Ag NPs. We have measured the dispersion stability, hydrodynamic sizes, and surface charges of Ag NPs using UV-Vis spectroscopy, dynamic light scattering (DLS) and Zeta-potential. We also performed flow cytometry (FCM) and inductively coupled plasma – mass spectrometry (ICP-MS) measurements to quantify cellular Ag NPs under various exposure conditions. Inhibitor assays on endocytosis mechanisms were also conducted and confirmed with flow cytometry (FCM) and bio-transmission electron microscopy (bio-TEM), which provided us useful insight on the cellular uptake mechanisms of Ag NPs in A549 cells.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-24**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:54, 좌장: 김병권

Physicochemical characterization of ZnO nanoparticles and their toxicity assessments using human lung epithelial cells(A549)

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Zinc oxide(ZnO) is one of the widely-used engineering nanoparticles(NPs), which is commonly used as ingredients of sunscreen or base make-up products to absorb UV radiation. In this study, Physicochemical characterization of ZnO nanoparticles (25, 50, and 150 nm) and their cellular association with human lung epithelial cells (A549) was investigated. For the ZnO nanoparticles with different surface charge and hydrodynamic size, single particle ICP-MS experiment was performed to obtain concentrations of ZnO particles and Zn2+ ion. MTT assay and flow cytometry (FCM) measurements were performed for A549 cells exposed to ZnO NPs for 24 hours. The measurement of side scattering (SSC) intensity in FCM is used as a method for the quantification of cellular ZnO NPs. Transmission electron microscope (TEM) was also used to observe the cellular association of ZnO particles. By using these integrated testing methods, we can provide better insights on the effect of ZnO NPs on biological systems.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-25**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:56, 좌장: 김병권

ISDD 모델링과 라만분광법을 이용한 탄소나노튜브의 effective dose 값 비교연구

채진만 윤태현[1,*]

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나노물질이 인체에 미치는 영향을 이해하기 위해서, 생체 외에서의 세포를 기반으로 한 실험이 행해지고 있다. 세포가 나노물질에 노출되었을 때, 이 나노물질이 세포에 직접적으로 전달되는 양을 'effective dose'라고 한다. 이 논문에서는 실용성이 뛰어난 물질로 알려진 탄소나노튜브(CNT)에 대하여 ISDD (in vitro sedimentation, diffusion and dosimetry) 모델링을 이용해서 구한 이론적인 effective dose 값과 라만분광법 실험을 이용해서 구한 실험적인 effective dose 값을 비교하여 ISDD 모델링의 실용성을 알아보고자 하였다. 우선 ISDD 모델링을 진행하기 위해서 고순도의 CNT 와 RPMI-full media 용매를 합친 샘플을 이용하였고, Effective dose 를 계산하기 위한 인자로 effective density 값을 얻기 위해서 VC(volumetric centrifugation) Method 을 사용하였다. Effective density 값등의 인자들을 ISDD 모델링의 식에 넣어주면 Effective dose 값에 해당하는 (number, surface area, mass) 값들을 구할 수 있다. 그리고 라만 분광법을 이용해서 침전된 CNT 의 양을 측정함으로서 effective dose 를 실험적으로 측정할 수 있으며, 결과적으로 구한 effective dose 측정값을 ISDD 모델링을 이용한 예측값과 비교를 함으로서 ISDD 모델링의 실용성이 있는 지 확인할 수 있었다.Reference: 1) Glen DeLoid et al, Nat. commun, 2014, 5, 35142) A.l. Lopez-Lorente et al, Analyst, 2014, 139, 290

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-26**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 09:58, 좌장: 김병권

Fabrication of Buckypaper using MWCNTs with Multivacancy Defects for Filtering Ultrafine Particulate Matter

송민우

수원대학교 신소재공학과

Our ultimate goal of this study is to fabricate buckypaper using multivacancy multi-walled carbon nanotubes (MWCNTs) for filtering ultrafine particulate matter application. First, MWCNTs-Co composites are fabricated by hydrothermal method and heat treatment in atmospheric conditions. Subsequently, cobalt oxide nanoparticles are removed by acid treatment. Through the processes, we can obtain multivacancy MWCNTs with high surface area. In addition, nitrogen-doped MWCNTs with multivacancy defects were obtained via chemical vapor deposition (CVD) method and the multivacancy MWCNTs were mixed with conducting polymer and ionic polymer. These surface modified and polymer composite MWCNTs with multivacancy defects are also employed to fabricate bukcypapes for filtering ultrafine particulate matter (PM 2.5). Here, we present the bukypapers using various multivacancy MWCNTs and filtration experimental data.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-27**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:00, 좌장: 김병권

Flow cytometry study of the influence of agglomeration on effective in vitro dosimetry and cellular association of silver nanoparticles

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Nanoparticles (NPs) are becoming increasingly important in various biological and medical applications, from imaging and diagnostics to therapeutics and regenerative medicine, which requires comprehensive knowledge on how NPs interact with biological systems. In vitro assays are simple, fast and inexpensive approach to investigate these interactions and have been very useful in providing insights into the cellular interaction of NPs. However, they still face several challenges regarding their accuracy and reproducibility. One of the challenges is the effective dosimetry for inhomogeneously dispersed chemicals, such as NP dispersions. The actual NP concentrations that reach the adherent cells' surface are often different from the administered value, and one of the reasons for this discrepancy is the agglomeration and sedimentation of NPs. Exposure of NPs to cell culture media typically induce agglomeration and cause changes in their effective size and density. These parameters play important roles in their sedimentation and diffusion processes, which strongly influence their effective dose and cellular associations. Therefore, it is necessary to study how agglomeration of NPs affects their effective dose and cellular association, so that accurate and reproducible assay results can be generated.The objective of this study is to investigate the influence of Ag NP agglomeration on their effective in vitro dosimetry and their association with human lung cancer cells (A549). To address the influences of NP agglomeration on effective in vitro dosimetry, hydrodynamic size and effective density of Ag NP agglomerates in cell culture media were measured by dynamic light scattering (DLS) and volumetric centrifugation method (VCM) respectively, and were then used to estimate the effective in vitro dose of NP dispersions using a computational model developed by DeLoid et al. Moreover, to evaluate the impact of NP agglomeration on the sedimentation and diffusion processes, A549 cells were exposed to Ag NPs in upright and inverted configurations. Flow cytometry (FCM) side scattering (SSC) intensity measurement was used to quantify cellular association of Ag NPs. In the FCM technique, the SSC signal, which is related to the inner complexity of the cells, was combined with inductively coupled plasma mass spectrometry (ICPMS) technique and used to evaluate the association level of Ag NPs in A549 cells. On the basis of these FCM SSC and ICPMS measurements, we demonstrated the influence of agglomeration on the sedimentation and diffusion processes of NPs, and thus on effective in vitro dosimetry and cellular association of Ag NPs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-28**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:02, 좌장: 김병권

mPE-MMR to increase sensitivity and accuracy in peptide identifications from co-fragmented tandem mass spectra

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Mass spectrometry (MS)-based proteomics, which uses high-resolution hybrid mass spectrometers such as the quadrupole-orbitrap mass spectrometer, can yield tens of thousands of tandem mass (MS/MS) spectra of high resolution during a routine shotgun proteomics experiment. Despite being a fundamental step in MS-based proteomics, the accurate determination and assignment of precursor monoisotopic masses to the MS/MS spectra remains difficult. The difficulties stem from imperfect isotopic envelopes of precursor ions, inaccurate charge states for precursor ions, and co-fragmentation of MS/MS spectra. Here, we describe a composite method of utilizing MS data to efficiently assign accurate monoisotopic masses to MS/MS spectra, including those subject to co-fragmentation and unassigned charge state. The method, “multiplexed post-experiment monoisotopic mass refinement” (mPE-MMR), consists of the following: multiplexing of precursor masses to assign multiple monoisotopic masses of co-fragmented peptides to the corresponding multiplexed MS/MS spectra, multiplexing of charge states to assign correct charges to the precursor ions of MS/MS spectra with no charge information, and mass correction for inaccurate monoisotopic peak picking. When combined with MS-GF+, a database search algorithm based on fragment mass difference, mPE-MMR effectively increases both sensitivity and accuracy in PSMs and peptide identification from complex high-throughput proteomics data compared to conventional methods.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-29**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:04, 좌장: 김병권

Novel tridoped TiO_2 nanoparticles with Er^{3+}-Yb^{3+}-Ce^{3+} for photodegradation of Rhodamine B

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Titanium dioxide (TiO_2) has been extensively used on photocatalyst applications, because it has relatively high photocatalytic actively, robust chemical stability, unexpensive and nontoxicity. However, TiO_2 has an energy band gap of about 3.2 eV due to the reason it mainly absorbs the ultraviolet portion of the solar spectrum and only a small amount of visible light. Thus, increasing photocatalytic efficiency by increasing light absorption ability of TiO_2 is necessary. In this study, Ce^{3+}, Er^{3+} and Yb^{3+} ions were doped simultaneously to TiO_2 for expanding light absorption range of TiO_2. The effects of synthetic temperatures, concentration of dopants in synthesis process of TiO_2 nanoparticles on photocatalytic efficiency for Rhodamine B were investigated. In addition, pH value of photodegradation medium was also optimized.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-30**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:06, 좌장: 김병권

Relationship between in vitro and in vivo toxicity of carbon nanotube: a meta-analysis from literature data

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As the number of nano-products has been sharply increasing in recent years, there are more and more public concerns about the safety of nanomaterial and related products. Generally, toxicity of nanoparticles is evaluated through in vitro (experiments with cultured cells) and in vivo (experiments with living organisms) protocols which require much time and labor cost. With the development of in silico approach (building and applying computational models for the toxicity prediction of nanomaterials), time and labor cost for the hazard assessment could be reduced [1]. The relationship between in vitro and in vivo toxicity has not been clear yet. Carbon nanotube materials have been used widely in industry and household and become a good object of studying that relationship. Gernand et al [4] already did meta-analysis on in vivo toxicity of multi-wall carbon nanotube and made a prediction model based on random forest algorithm. In this study, we used Gernand data as main source of in vivo toxicity data of carbon nanotube and collected in vitro toxicity data from other literatures and did meta-analysis to find out relationships between in vitro and in vivo toxicity of carbon nanotube materials. This study will support for later research of correlating in vivo and in vitro toxicity of nanomaterials.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-31**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:08, 좌장: 김병권

Highly selective determination of catecholamines using dithiol modified upconversion nanoparticles with metal ions

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창원대학교 화학과

Catecholamines are a well-known neurotransmitter and related mammalian central nervous system. Therefore, when the amount of catecholamines in tissues are abnormal, it is possible to cause several diseases including Parkinson’s diseases, chronic inflammatory diseases. However, catecholamine-secreting cells are converted tyrosine to L-DOPA and then to dopamine. Furthermore, epinephrine and norepinephrine are released by dopamine. Dopamine, epinephrine, and norepinephrine show different action in the nervous system, although all catecholamines are conducted both as hormone and neurotransmitter. Therefore, separation of catecholamines is required with highly sensitivity, simple, and fast analytical method. Upconversion nanoparticles (UCNPs), that convert near-infrared radiation (NIR) to visible, have been used the biological field. Furthermore, NIR irradiation has deeper penetration properties and less harmful to biological samples compared to UV excitation. Therefore, our goal is a determination for catecholamine respectively with various metal ions by upconversion luminescence (UCL). First, we developed a facile synthesis of Yb^{3+}/Er^{3+}-doped $NaLuGdF_4$ (UCNPs) coated with 1,2-ethanedithiol (EDT) to detection of catecholamines. Second, metal ions decorated UCNPs are conducted to the separation of dopamine and epinephrine from catecholamines.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-32**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:10, 좌장: 김병권

Copper Coordinated Cationic Polyvinylpyrrolidone as a Novel Fluorescent Probe for Hydrogen Sulfide in Aqueous Solution

ABDELAAL ALI Salah Mahmoud Tawfik Ahmed 이승하 이용일*

창원대학교 화학과

A cationic polyvinylpyrrolidone (Cat-PVP) was prepared via Claisen- Schmidt condensation in super basic media and characterized using different spectra analyses (IR and ^{1}H-NMR). The prepared Cat-PVP was utilized to prepare a stable fluorescence copper coordinated cationic polyvinylpyrrolidone in aqueous media. The Cu-CatPVP was successfully utilized to detect hydrogen sulfide (H_2S) based on strong affinity between sulfur and copper. The quenching effect on the fluorescence intensity of the Cu-CatPVP probe showed very good linearity with H_2S concentrations in the range of 1−40μM, with detection limit as low as 0.13 μM. The presented probe promising selectivity toward H_2S over anions, biothiols as well as other amino acids in neutral media and was successfully applied for detecting the H_2S in real samples.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-33**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:12, 좌장: 김병권

Upconversion Nanoparticles Functionalized with Novel Amphiphilic Polymers for Enhanced Biocompatibility and Bioimaging of KB Cells

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창원대학교 화학과

We have synthesized amphiphilic alginate (Al-NH-PEG-NH_2 and Al-NH-PEG-NH-FA)as the novel ligands to functionalize upconversion luminescent surface. Upconversion nanoparticles ($NaLuGdF_4$: Yb,Er,Cr) were capped with a thin polymer shell by replacing the oleate ligand of hydrophobic UCNPs by multidentate carboxylates of amphiphilic alginate polymers. Using amphiphilic alginate polymers as the surface ligands not just enhances the stability and biocompatibility of the UCNPs under physiological conditions but also displayed enhanced upconversion luminescent intensity. It was found that a maximum upconversion luminescence enhancement of 20-fold was obtained in comparison with the hydrophobic UCNPs. In order to demonstrate the targeted bioimaging capability of the functionalized-UCNPs, two cell lines (KB and HeLa) were employed for the investigations on the basis of their different folate receptor expression level. The results illustrated that the UCNP-Al-NH-PEG-NH-FA was specific in targeting KB cell lines more than HeLa cell lines under an excitation wavelength of 980 nm. The cell viability of two types of cells incubated with high concentration (300 $\mu g \cdot mL^{-1}$) of functionalized-UCNPs still remained above 85% after 24 h. The formation of stable water-dispersible UCNPs with enhanced emission, together with their amphiphilic and biocompatible polymer coating, is promising for building multifunctional nanostructures for cell imaging, therapy, and drug delivery.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-34**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:14, 좌장: 김병권

Ultrasensitive fluorescence detection of heparin using CdTe quantum dots coated with amphiphilic polythiophenes

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A new strategy for the detection of heparin is developed by utilizing quantum dots (QDs) coated with amphiphilic polythiophenes. The amphiphilic polythiophenes (PTPQ2000)-coated CdTe QDs were synthesized by in situ polymerization of modified thiophene on the surface of CdTe QDs. The PTPQ2000-coated CdTe QDs has a tremendously enhanced fluorescence and improved biocompatibility compared to the uncoated CdTe QDs. The PTPQ2000-coated CdTe QDs was successfully utilized to detect heparin. The emission of PTPQ2000-coated CdTe QDs is found to be quenched upon addition of the polyanionic heparin, due to electron transfer via electrostatic and/or hydrogen bonding interactions between heparin and PTPQ2000-coated CdTe QDs. The fluorescence intensity quenched with the increase of heparin and a good linear relationship was observed for heparin detection in buffer solution and the limit of detection (LOD) is 0.75 nM. The selectivity results of the fluorescence assay revealed that our system displayed excellent fluorescence selectivity towards heparin over its analogues. This fluorescence "switch of" assay for heparin is label-free, less toxic, sensitive and selective, which can be used to detect heparin in biological systems.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-35**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:16, 좌장: 김병권

Phospholipase A2-responsive UCNPs-loaded Phosphate Micelles for Prostate Cancer Cells Imaging

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창원대학교 화학과

Rare-earth upconversion nanoparticles (UCNPs) have been proposed as biological luminescent labels for the bioimaging application. However, their toxicity, low dispersion, and low selectivity call into question their suitableness in nanomedicine. Herein, UCNPs-loaded phosphate micelles formed from the secreted phospholipase A2 (sPLA-2) enzyme cleavable phosphate micelles to deliver UCNPs directly to prostate cancer cells has been reported. These phosphate micelles were designed from biocompatible materials. Through a dye micellization method, the CMC value of micelles was determined to be 6.38×10^{-4}M. The activity of (sPLA-2) enzyme toward the synthesized micelle was investigated and confirmed using LC-MS. TEM results showed that micelles have a size ranged between 50 to 80 nm; whereas UCNPs loaded micelles have from 60 to 100 nm. Bio-imaging experiments conducted on KB, HeLa, and 22Rv1 cell lines confirmed the selectivity of UCNPs-loaded micelles toward 22Rv1 cell line. Moreover, the non-selective binding of UCNPs towards cells with low expression of PLA-2 was significantly reduced and MTT assay results confirmed the biocompatibility of micelles.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-36**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:18, 좌장: 김병권

Identification of C_{18} Ceramide with Metal Ions using Electrospray Ionization Mass Spectrometry

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Herein, electrospray ionization – mass spectrometry [ESI-MS/MS] is applied for the investigation of C_{18} – ceramide complexes with transition metal ions such as Mn^{2+}, Cu^{2+}, Co^{2+} and Ni^{2+}. The formation and fragmentation of doubly charged cluster ions of C_{18} – ceramide with metal ions will be studied by ESI-MS/MS in the positive mode. Tube lens offset voltage and concentrations of C_{18} – ceramide and metals are optimized to determine the best conditions for charged ions. The fragmentation pathways of metal ion complexes with C_{18} – ceramide and the compositions of these complexes are determined by collision induced dissociation (CID). All metal ions show the similar complexation with C_{18} ceramide. Consequently, MS/MS combined with ESI can be the most powerful technique to scrutinize transition metal ion complexes with C_{18} – ceramide. Experiments on metal cations have mostly been restricted to singly charged ions due to the significant experimental challenges in interpreting the structure and chemistry of multiply charged metal complexes, strongly suggests the need for studies using ESI-MS/MS.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-37**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:20, 좌장: 김병권

Facile synthesis of $NaYF_4$:Yb^{3+}/Tm^{3+} upconversion nanoparticles coated with polyepinephrine for optosensing of Fe^{3+} ion

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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+}/Tm^{3+} doped $NaYF_4$ UCNPs coated with polyacrylic acid (PAA) was accomplished by the one-step hydrothermal method. Then polyepinephrine (PEP) formed on the UCNPs via self-polymerization of epinephrine. After polymer coated UCNPs showed enhancement of upconversion luminescence (UCL), and optimize condition was found. The successful synthesis of $NaYF_4$:Yb^{3+}/Tm^{3+}@PEP was used for optosensing of the Fe^{3+} ion. In detail, luminescence properties and morphology were discussed. From the obtained results, could be concluded that $NaYF_4$:Yb^{3+}/Tm^{3+}@PEP was successfully synthesized by the one-step hydrothermal approach, which is detected Fe^{3+} ion in aqueous system with high selective, sensitive, and simple. Furthermore, the $NaYF_4$:Yb^{3+}/Tm^{3+}@PEP showed relatively high cell viability. The high-quality of the synthesized UCNPs have prominent potential applications for optical nanodevices, bioimaging, and bioanalytic sensing.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-38**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:22, 좌장: 김병권

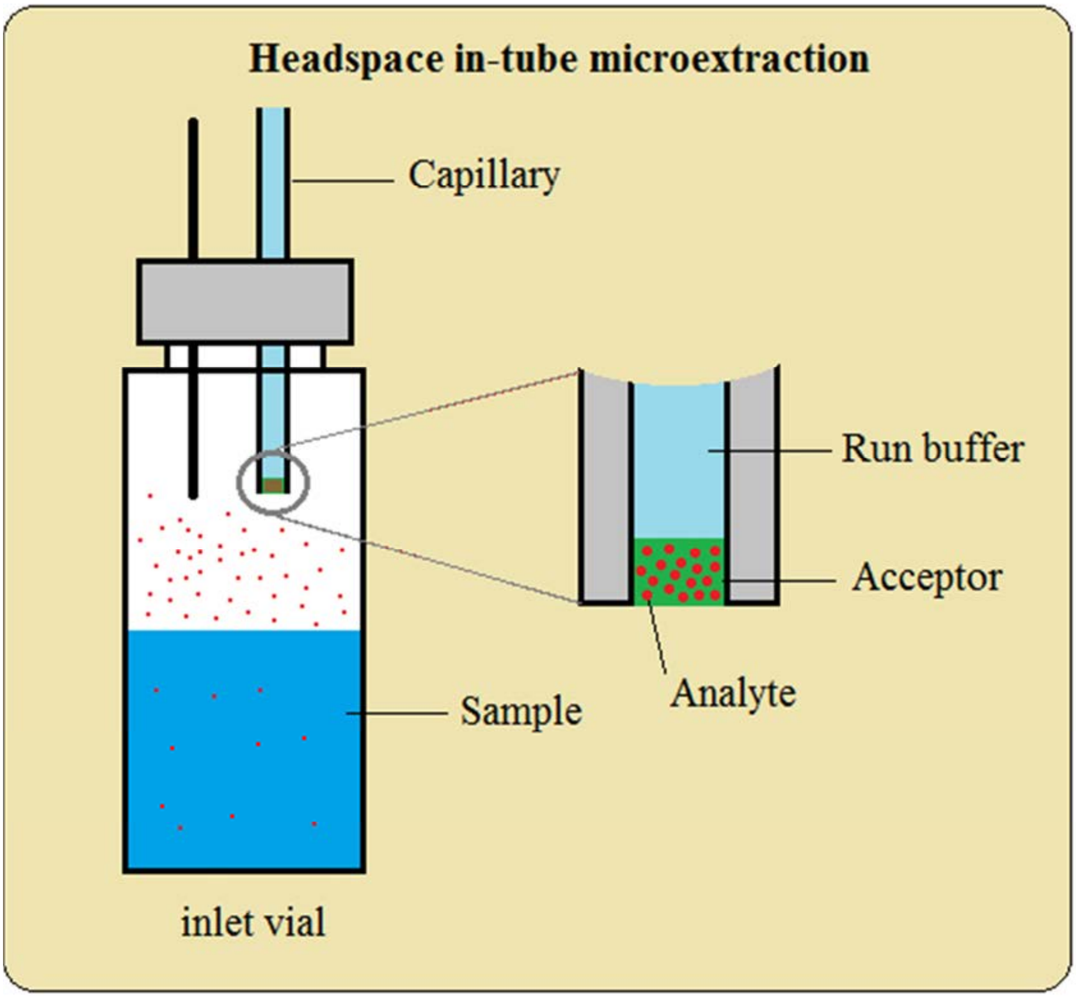
Determination of trichlorophenols in water samples using headspace in-tube microextraction followed by capillary electrophoresis

karimi maryam 정두수*

서울대학교 화학부

Chlorophenols are used widely in industry as intermediates in the production of dyes, plastics and pharmaceuticals, and are commonly found in pulp and paper mill wastewater, which pollute the groundwater sources. The harmonization of the analysis of chlorophenols in water is of importance due to the toxicity of these components and the presence in the aquatic environment. In the previous research, we demonstrated a fast simple preconcentration and microextraction method, head space in-tube microextraction (HS-ITME), which was initially used for determination of chlorophenols (CPs) and BTEX (benzene, toluene, ethylbenzene, and m-xylene) in wine and water samples, respectively. Rapidity, high enrichment factor, simplicity of operation and low cost are some of the advantages of this method. In this study HS-ITME is applied to determine six trichlrophenols in a water sample. At first, an acceptor phase was injected into the capillary in a desired duration of time. The capillary inlet is placed in the headspace above an acidified donor solution; volatile acidic analytes were extracted into the acceptor phase (a basic solution) in the capillary. After extraction, the analytes enriched in the basic acceptor plug were analyzed with capillary zone electrophoresis.

Some effective parameters on extraction, such as donor volume, donor pH, type of acceptor and its volume, waiting time, pre-injection volume, salt addition, extraction time and temperature were investigated. Also, the influence of adding organic additives on the headspace analysis of trichlorophenols is investigated.


Headspace in-tube microextraction
Capillary
Run buffer
Acceptor
Analyte
Sample
inlet vial

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-39**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:24, 좌장: 김병권

MATLAB-based Statistical Analysis Software for Edible Oils Classification

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서강대학교 화학과

Edible oils contain a variety of lipids, particularly diacylglycerols (DAGs) and triacylglycerols (TAGs). Different edible oils have their own signature lipid distribution. In this study, we acquired MALDI-TOF (Tinkerbell, Asta, Korea) mass spectra of 9 species of edible oils, such as sesame, perilla, olive, canola, grape-seed, sunflower-seed, corn, soybean, coconut oils. For the classification of edible oils using statistical analysis, we used principle component analysis (PCA), partial least square-determinant analysis (PLS-DA) and support vector machine (SVM). Using these statistical methods, statistical models were established. Based on those statistical analysis results, an edible oil analysis software was constructed using MATLAB. This software can not only visualize the acquired MALDI mass spectrum, but also readily classify unknown edile oils based on the PCA/PLS-DA/SVM statistical models by projecting the acquired spectrum components onto the established statistical models for the classification of edile oils.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-40**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:26, 좌장: 김병권

MALDI-TOF/TOF applications of TEMPO-assisted free radical initiated peptide sequencing (FRIPS) mass spectrometry

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Unlike CID-based peptide sequencing, TEMPO-assisted FRIPS makes use of a radical species for peptide sequencing. In this method, a peptide is conjugated with o-TEMPO-Bz-C(O)-NHS and thus generating o-TEMPO-Bz-C(O)-peptides. When o-TEMPO-Bz-C(O)-peptides is subjected to collisional activation, o-TEMPO-Bz-C(O)-peptides undergoes homolytic cleavage, forming ·Bz-C(O)-peptide. Then·Bz-C(O)-peptide produces a, c, x, and z-type products upon the secondary collisional activation. So far, ESI has been used for the TEMPO-assisted FRIPS MS. In this study, MALDI-TOF/TOF was performed on o-TEMPO-Bz-C(O)-peptides. It was revealed that MALDI ionization for o-TEMPO-Bz-C(O)-peptides was greatly affected by the matrix. 3-HPA(3-Hydroxypicolinic acid) was found to be a good matrix, whereas DHB, CHCA, showed a very low ionization efficiency. MALDI MS/MS of the detected o-TEMPO-Bz-C(O)-peptides yielded a, c, x and z-type products.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-41**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:28, 좌장: 김병권

Development of a Dissolved Organic Matters (DOMs) Analysis Program Using a MATLAB Language

장인애 오한빈*

서강대학교 화학과

Dissolved organic matters (DOMs) is a complex mixture of degradation products from plants and animals and it plays a key role in the global carbon cycle. The ultra-high resolution mass spectrometer, such as Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS), is required to analyze DOMs in a river or ocean. Because the number of DOMs that exist in the mass spectrum is at least over 2000 peaks, an automatic analysis software is needed for the analysis of the numerous peaks of DOMs. Thus, we developed a software for the analysis of DOMs using a MATLAB language. In this study, we collected water samples of the Han River at Amsa located in the main stem and Jungnang located in the tributary. The collected water samples divided into two microtubes, and then one was treated C18 solid phase extraction (SPE) and the other was subjected to C18 SPE after microbal incubation for 5 days. Mass spectra were obtained by 15 T FT-ICR MS (SolariX XR, Bruker Daltonics, Germany) and various Van Krevelen diagrams were plotted using a home-coded MATLAB program. To conclude, the Han River of Amsa and Jungnang water samples were analyzed by a semi-automatic home-coded program, and a graphic user interface (GUI) will be added in the near future.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-42**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:30, 좌장: 김병권

Make Your Own Nano-LC MALDI Spotter Robot using a 3D Printer

이재웅 오한빈*

서강대학교 화학과

The 3D printing technology is growing very rapidly, and is bringing about significant advances in many research areas. On the 3d printing related website, the stories of making 3d printed parts and custom equipment have been posted. In this research, we made a DIY nano-LC MALDI spotter robot using 3D printed custom parts. Using this equipment, nano-LC and MALDI matrix loading can be conveniently coupled online and thus the separated eluents from nano-LC can be loaded automatically onto the MALDI plate. This DIY robot was made of only 3d printed parts and the parts on the online marketplace, so that anyone can make it and carry out maintenance easily and inexpensively. In this DIY robot, the loading speed can be readily controlled using a home-coded software. In addition, a camera is equipped so that the loading process can be monitored.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-43**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:32, 좌장: 김병권

Improved Performance of Dye-sensitized Solar Cell in Counter Electrode Using Upconverting Capability in Ln-FTO and FTO-UCNP Hybrid Nanostructures

NGUYEN THI THU THUY **B.T.Huy** 이용일*

창원대학교 화학과

Upconverting capability of hybrid nanostructure is promising potential candidate to dye-sensitized solar cell because of their unique properties to enhance of near-infrared light harvesting. In this paper, we reported a novel Ln-FTO and FTO-UCNP hybrid nanostructures and investigated their excellent optical and catalytic capability for using as the counter electrode in dye-sensitized solar cell (DSSC). FTO based on F-doped SnO_2 was used as special catalyst with excellent chemical stability, and high efficiency for counter electrode materials in dye-sensitized solar cell. These observations by IPCE and SPS demonstrated high effect Near-infrared light to electricity to upconversion counter electrode, even than Pt electrode in terms of low cost, simple preparation and high solar-to-electric power conversion efficiency (PCE). We proved that this novel upconversion hybrid nanostructure opened new era to excellent materials in dye-sensitized solar cell with upconvertiong capability, decent catalytic properties, and good conductivity.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-44**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:34, 좌장: 김병권

Glycan Heterogeneity Differentiation Using Lectin-based SDC Separation and Glycopeptide level SDC Separation

<u>정미선</u> 조원련*

원광대학교 바이오나노화학부

Previous work in this group showed displacement phenomena in lectin affinity chromatography in glycoprotein level using LEL Lectin-based SDC Separation. However, the SDC can fail to differentiate between glycoforms of proteins with multiple glycosylation sites when a high affinity glycan is conjugated to a protein at one site and a low affinity glycan at another site in the same protein. The high affinity glycan will dominate binding of the protein to the lectin column and the low affinity glycan will be unrecognized. This problem can be solved with the digestion of the glycoproteins using self-packed trypsin column and glycopeptide Lectin-based SDC Separation. Human pooled plasma were digested with the self-packed trypsin columns without chemicals.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

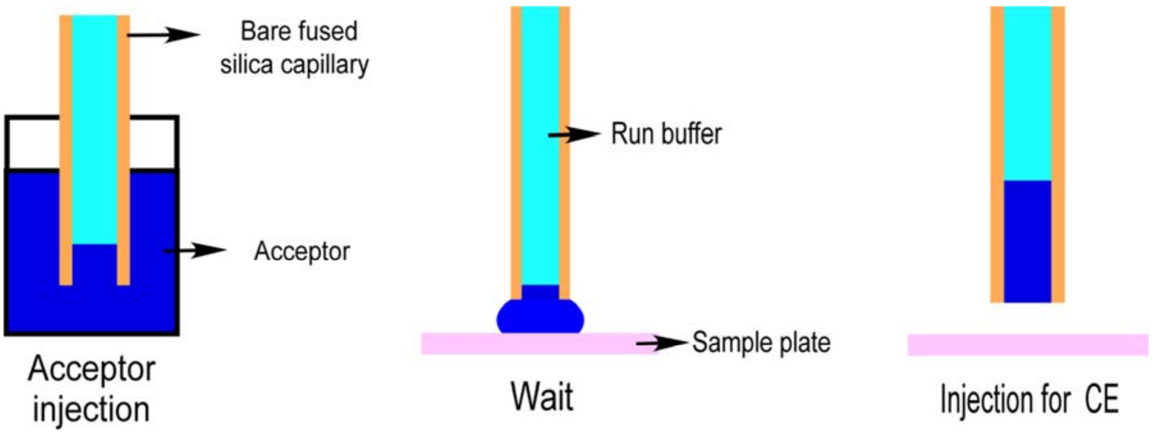
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-45**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:36, 좌장: 김병권

Liquid extraction surface analysis coupled with commercial capillary electrophoresis for direct analysis of solid surface samples rapidly

정선경 정두수[1,*]

서울대학교 화학부 [1]서울대학교 화학부

Capillary electrophoresis (CE) is well suited for the analysis of analytes in aqueous solutions. It is not easy to analyze a solid sample with CE since labor-intensive sample pretreatment processes are required. For example, a solid sample should be grounded, homogenized, centrifuged, extracted into an organic solvent, and then reconstituted into an aqueous solution suitable for CE. So we used liquid extraction surface analysis (LESA) that extracts chemicals on the surface of various solid samples without any sample pretreatment. Dried analytes doped on a surface were directly extracted to a hanging drop of extractant at the inlet tip of a capillary. After extraction, a small volume of acceptor was injected into the capillary and analyzed by a commercial CE instrument. LESA-CE was used to determine three species of insecticides, chlorantraniliprole, kresoxim-methyl, and pyraclostrobin. The U.S. Environmental Protection Agency (EPA) limits the allowable amounts of the insecticides to 4.0 ppm, 0.5 ppm, and 2.5 ppm respectively. For these water-insoluble analytes, micellar capillary electrophoresis (MEKC) was used and an on-line stacking method, analyte focusing by micelle collapse (AFMC) was combined to enhance the sensitivity. These three pesticides doped on sample plate were extracted with the inlet of a capillary and analyze directly with CE. Several parameters such as the condition of AFMC-MEKC, composition of acceptor, extraction time were optimized. The limits of detection (LODs) with LESA-AFMC-MEKC were 72, 23, and 29 ppb, respectively. Thus LESA-CE is a simple, sensitive and more rapid method for the analytes solid surface analytes without any pretreatment processes required for conventional analysis methods. The developed LESA-CE of high spatial resolution and immediate quantification ability is promising for the analysis of biological surfaces of cells and tissue, or even technical surfaces.


Bare fused silica capillary
Acceptor
Acceptor injection
Run buffer
Sample plate
Wait
Injection for CE

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-46**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:38, 좌장: 김병권

Real-Time Kinetic and Mechanistic Study of Decarboxylation Reaction of Pyruvic Acid using Hyperpolarization Technique

서형림 황수민 이영복*

한양대학교 바이오나노공학과, 응용화학과

Kinetic and mechanistic study of fast chemical or biochemical reactions is one of the major applications of NMR spectroscopy. In order to characterize the reactions, low-temperature NMR technique is traditionally utilized. However, the low-temperature technique is very limited to specific reactions due to solvent and solubility issues. Here, we demonstrate room-temperature kinetic and mechanistic study of decarboxylation reaction of pyruvic acid using dynamic nuclear polarization (DNP) technique. Hyperpolarization of pyruvic acid provides a sufficient signal-to-noise ratio for real-time detection of 13C NMR signals as the reaction progresses. This capability enables DNP method to be an attractive method for both kinetic and mechanistic study of various chemical or biochemical reactions.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-47**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:40, 좌장: 김병권

Silicon Nanoparticle based Magnetic Resonance Imaging Probe for Early-Stage Cancer Diagnosis

최익장 김도경 이영복*

한양대학교 바이오나노공학과, 응용화학과

Silicon-based nanoparticle has been attracting lots of interest in the field of magnetic resonance (MR) applications because of its specific features of biocompatibility and flexible surface chemistry. Since a core region of the crystalline Si NPs is mostly protected from paramagnetic centers on its surface defect sites, the Si NPs conventionally represent extremely long depolarization times, resulting in high MR signal-to-noise ratio with minimum background signals. In order to synthesize size-controlled Si NPs, we utilized magnesiothermic reduction of silica nanoparticles at various reduction temperature and time. In addition to the traditional synthetic approach, we produce 29-silicon enriched NPs with synthesized 29Si-TEOS for the purpose of additional signal enhancements. The enriched Si NPs in combination with hyperpolarization technique provide sufficient MR signals for *in vitro* and *in vivo* MR applications.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL2.O-48**
발표분야: Oral Presentation of Young Analytical Chemists Ⅱ
발표종류: 구두발표, 발표일시: 금 10:42, 좌장: 김병권

Characterization of heterogeneous oligomerization of amyloid-β 1-40 and 1-42 using electrospray ionization mass spectrometry

허채은 김준곤*

고려대학교 화학과

Amyloid fibrillation of amyloid-β (Aβ) peptides has been accepted as the main cause of Alzheimer's disease (AD). Aβ40 is the most abundant form in Aβ peptides, while Aβ42 is highly relevant to the progress of AD. The ratio of Aβ40:Aβ42 in human brain is approximately 9:1, but the ratio of Aβ42 is increased in the brains of patients with AD. Since Aβ42 is more aggregation-prone than Aβ40, amyloid fibrillation of Aβ peptides can be promoted when increasing the ratio of Ab42. Additionally, it has been reported that the high ratio of Aβ40 inhibits the aggregation of Aβ42. However, the molecular interaction between Aβ40 and Aβ42 during the inhibition of Aβ42 fibrillation is still unclear. In this research, we demonstrate the role of Aβ40 during the fibrillation process of Aβ42. We monitored the fibrillation process of Aβ42, Aβ40 and their 1:1 mixtures using thioflavin T (ThT) assay and electrospray ionization mass spectrometry (ESI-MS). Then, we further investigated the changes in gas-phase structures of homo- and hetero- oligomers of Aβ40 and Aβ42 using ion mobility spectrometry (IMS) combined with ESI-MS. Our results suggest that Aβ40 delays the nucleation process of Aβ42 by forming the hetero-oligomers, and overall rates in the fibrillation kinetics are decreased.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL2.O-49**

발표분야: Oral Presentation of Young Analytical Chemists Ⅱ

발표종류: 구두발표, 발표일시: 금 10:44, 좌장: 김병권

[발표취소] 확산이 제한된 하이드로젤 입자 내에서 핵산증폭반응 효율연구

임혜원 김원진[1] 김상경[2,*]

한국과학기술연구원(KIST) 바이오마이크로시스템연구단, 경희대학교 응용화학과, 경희대학교 유전공학과 [1]한국과학기술연구원(KIST) 바이오마이크로시스템연구단, 경희대학교 응용화학과 [2]한국과학기술연구원(KIST) 바이오마이크로시스템연구단

발 표 취 소

본 논문은 발표취소된 논문입니다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.O-6**
발표분야: Bioconjugation
발표종류: 분과기념강연, 발표일시: 목 10:10, 좌장: 정상전

Cell penetrating peptides as delivery tools for intracellular modulators in their nano-molar scale

유재훈

서울대학교 화학교육과

Cell penetrating peptides (CPP) are attractive tools to deliver non-soluble small molecule or biological modulators, which are difficult to get into cells by themselves. Since Tat peptide was known as the first CPP from viral source in 1980's, more than 200 kinds of CPPs has been reported. Most of them, however, deliver conjugated modulators at their micro-molar concentrations. Those high concentrations of CPPs make us reluctant to use as deliver tools of nano-molar-affinity modulators against intracellular targets, because micro-molar scales of modulators cause unwanted adverse effects and cytotoxicy. In order to address this concentration issue, we have been developing CPPs that can deliver a variety of small molecule or biological modulators in their nanomolar concentrations.[1] Since high helical contents of double bundled amphipathic peptides connected by two disulfide bonds can penetrate into cells in low nano-molar concentrations, we can deliver the conjugated small molecules or large biological modulators that is simply complexed with CPPs. Examples of the delivery are discussed, showing that our nano-scale CPPs are efficient tools to deliver small molecules as well as biological molecules using cell-based assays and animal models as well.

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(3) Jang S, Hyun S, Kim S, Lee S, Lee IS, Baba M, Lee Y, Yu J. Angew Chem Int Ed Engl. 2014, 53(38):10086-9.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.O-1**

발표분야: Bioconjugation

발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 우주랑

Sin3A: A transcriptional corepressor in the regulation of neurogenesis

HALDER DEBASISH* 신인재[1,*]

연세대학교 화학 [1]연세대학교 화학과

Sin3 is a transcriptional corepressor for REST silencing machinery that represses multiple neuronal genes in non-neuronal cells. However, functions of Sin3 (Sin3A and Sin3B) in suppression of neuronal phenotypes are not well characterized. Herein we show that Sin3A knockdown impedes the repressive activity of REST and enhances differentiation of pluripotent P19 cells into electrophysiologically active neurons without inducing astrogenesis. It is also found that silencing Sin3B induces neurogenesis of P19 cells with a lower efficiency than Sin3A knockdown. The results suggest that Sin3A has a more profound effect on REST repressive machinery for silencing neuronal genes in P19 cells than Sin3B. Furthermore, we show that a peptide inhibitor of Sin3A-REST interactions promotes differentiation of P19 cells into functional neurons. Observations made in studies using genetic deletion and a synthetic inhibitor suggests that Sin3A plays an important role in the repression of neuronal genes by the REST regulatory mechanism.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.O-2**
발표분야: Bioconjugation
발표종류: 구두발표, 발표일시: 목 09:10, 좌장: 우주랑

Structural and Mechanistic Insights into Development of Chemical Tools to Control Individual and Inter-Related Pathological Features in Alzheimer's Disease

이혁진 임미희[1,*]

UNIST 생명과학연구부 [1]UNIST 자연과학부/화학과

To elucidate the involvement of individual and inter-related pathological factors [i.e., amyloid-β (Aβ), metals, and oxidative stress] in the pathogenesis of Alzheimer's disease (AD), chemical tools have been developed. Characteristics required for such tool construction, however, have not been clearly identified; thus, the optimization of available tools or new design has been limited. In this presentation, we will present key structural properties and mechanisms that can determine tools' regulatory reactivities with multiple pathogenic features found in AD. A series of small molecules was built up through rational structural selection and variations onto the framework of a tool useful for in vitro and in vivo metal–Aβ investigation. Variations include: (i) location and number of an Aβ interacting moiety; (ii) metal binding site; and (iii) denticity and structural flexibility. Detailed biochemical, biophysical, and computational studies were able to provide a foundation of how to originate molecular formulas to devise chemical tools capable of controlling the reactivities of various pathological components through distinct mechanisms. Overall, our multidisciplinary investigation illustrates that a structure-mechanism-based strategy can assist in significantly advancing the rational tool invention for such a complicated brain disease.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.O-3**
발표분야: Bioconjugation
발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 우주랑

Development of a Stapled Peptide Inhibitor Targeting NCoA1/STAT6 Interaction

이영주 임현석*

POSTECH 화학과

Signal transducer and activator of transcription 6 (STAT 6) is a member of STAT family. It takes a critical role in immune response that involves in IL-4/IL-13 signaling after the binding with the essential coactivator NCoA1. However, abnormally activated STAT6 can increase inflammation signaling and lead to disease such as asthma. The conventional approaches to decrease inflammation signaling were to block either IL-4/IL-13 signaling factor. Instead, we focused on the NCoA1/STAT6 interaction which can block both IL-4/IL-13 signaling. The interaction between NCoA1 and STAT6 is mediated by LXXLL motif which acts as alpha helix recognition motif. Here in, we developed series of compounds that mimic the helical region of STAT6 protein by adopting ring closing metathesis method with Grubb's catalyst and Dibromo-xylene stapling method to inhibit the NCoA1/STAT6 interaction. Among these compounds, SS2 provides 10 times increased binding affinity compared to the non-stapled native peptide. In addition, it has much improved serum stability and cell permeability. SS2 disrupts NCoA1/STAT6 interaction in cellular level and decrease the transcriptional activity mediated by STAT6. In this study, we discovered the first-in-class NCoA1/STAT6 inhibitor that binds to NCoA1 competitively and disrupts NCoA1/STAT6 interaction. We expect that SS2 can be an effective NCoA1/STAT6 interaction inhibitor, and can further be a potential therapeutic candidate.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.O-4**

발표분야: Bioconjugation

발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 우주랑

Current status and technological trends in the development of antibody-drug conjugates

이선배

(주)알테오젠 R&D center

Antibody-drug conjugates (ADCs) elicit cancer-cell specific cytotoxicity by delivering highly potent drugs selectively to antigen-expressing tumor cells. Various parameters must be considered in designing optimal ADC construct, such as optimal drug-to-antibody ratio, conjugation method, cytotoxic payloads, and antigen specific mAb. Recent advance and technological trends in this field will be presented.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.O-5**
발표분야: Bioconjugation
발표종류: 구두발표, 발표일시: 목 09:50, 좌장: 우주랑

Design of the Well-Defined Antibody-Drug Conjugates (ADCs) :Preclinical Development of an anti-HER2 ADC, LCB14-0110

송호영

(주)레고켐 바이오사이언스 신약연구소

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 shows 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.

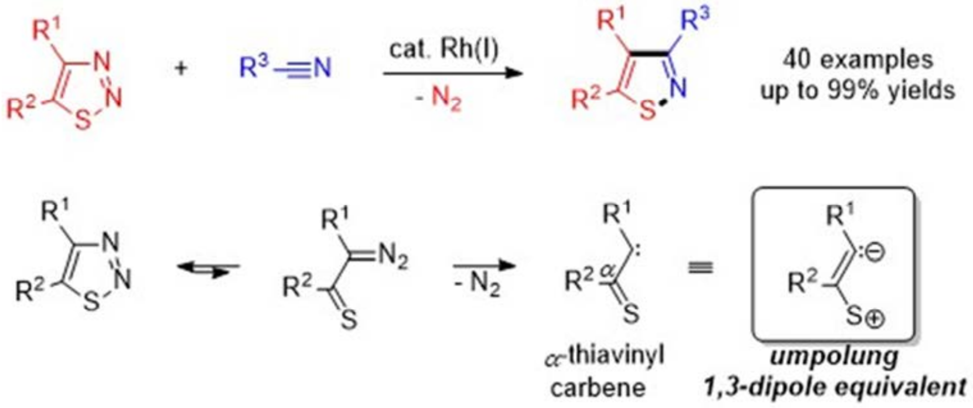
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.O-1**
발표분야: Oral Presentations of Young Scholars in Organic Division
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 박진균

Synthesis of Isothiazole *via* the Rhodium-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Nitriles

서보람 이필호*

강원대학교 화학과

Isothiazoles are valuable structural motifs found in many natural products, pharmaceutical compounds, and functional materials. For this reason, streamlined methods for their synthesis from readily available compounds must be developed.Herein, we developed a synthetic method for obtaining a wide variety of isothiazoles by the Rh-catalyzed transannulation of 1,2,3-thiadiazoles with alkyl, aryl, and heteroaryl nitriles, which proceeds *via* an α-thiavinyl Rh-carbenoid intermediate. The results suggest that during its reaction with nitriles, the α-thiavinyl carbene acts as an umpolung 1,3-dipole equivalent, in contrast to its behavior during its reaction with alkynes. The developed method was successfully employed to synthesize pentaoligomeric arylene compounds consisting of three benzene and two isothiazole rings.



일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.O-2**

발표분야: Oral Presentations of Young Scholars in Organic Division

발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 박진균

Development of Paper-Based Colorimetric Sensor System for the High-Throughput Screening of Ir-catalyzed C-H Borylation

김한성 엄민식[1] 한민수[1,*] 이선우[*]

전남대학교 화학과 [1]GIST 화학과

A paper-based colorimetric sensor system (PBCSS) was developed to analyze the amount of bis(pinacolato)diboron (B_2Pin_2) and applied as a high-throughput screening protocol in Ir-catalyzed C-H borylation. First, ninety-six ligands were screened for the borylation of benzene, and then twelve of them were selected and tested for five substrates. These reaction mixtures were spotted in the PBCSS, showing a blue-violet color. The value of the gray scale of each reaction was obtained from these colored spots and converted to the extent of conversion of B_2Pin_2. The extents of conversion of B_2Pin_2 obtained from the PBCSS showed good correlation with those obtained from gas chromatography analysis. In addition, the modified conversion using blank data showed good correlation with the yield of products.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)

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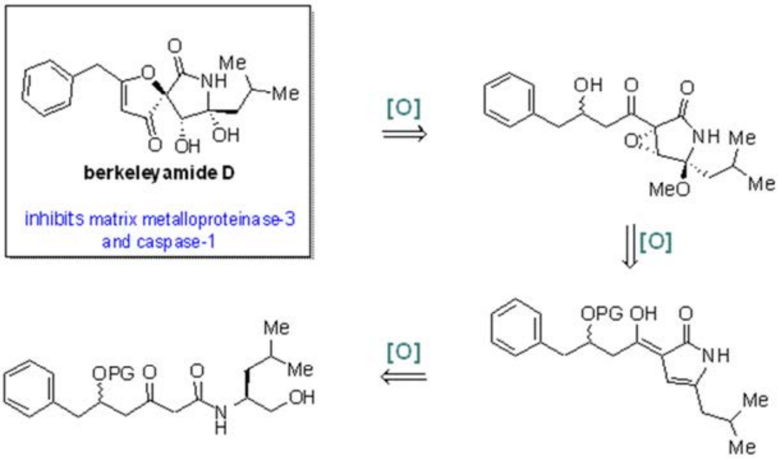
Biomimetic Total Synthesis of Berkeleyamide D

조덕희 한순규*

KAIST 화학과

Biomimetic total synthesis of berkeleyamide D is described. In 2004, Snider and Neubert reported a novel biomimetic route to 3-acyl-5-hydroxy-3-pyrrolin-2-ones.1 Inspired by this biomimetic sequence, our group envisioned a biosynthetically inspired total synthesis of berkeleyamide D. We sought to construct the oxa-azaspirocyclic core of berkeleyamide D from a linear precursor via a series of oxidation processes. Our synthetic strategy forms the basis for the synthesis of various natural products which contain the oxa-azaspirononenedione core.



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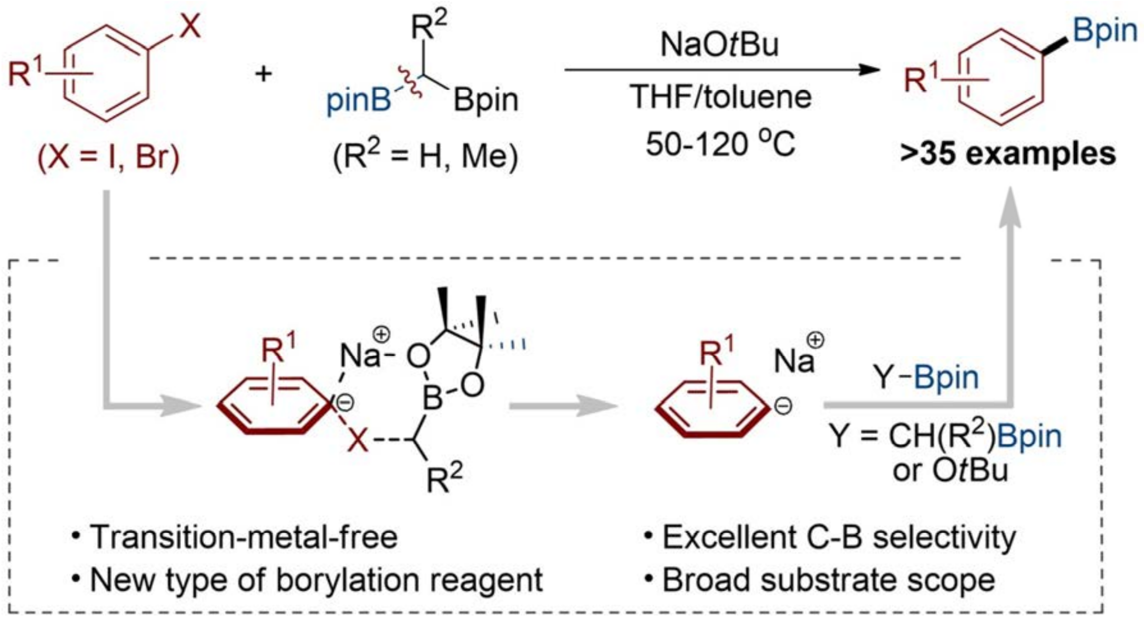
Chemoselective Coupling of 1,1-Bis[(pinacolato)boryl]alkanes for the Transition-Metal-Free Borylation of Aryl and Vinyl Halides: A Combined Experimental and Theoretical Investigation

이여산 조승환*

POSTECH 화학과

A new transition-metal-free borylation of aryl and vinyl halides using 1,1-bis[(pinacolato)boryl]alkanes as boron sources is described. In this transformation one of the boron groups from 1,1-bis[(pinacolato)boryl]alkanes is selectively transferred to aryl and vinyl halides in the presence of sodium *tert*-butoxide as the only activator to form organoboronate esters. Under the developed borylation conditions, a broad range of organohalides are borylated with excellent chemoselectivity and functional group compatibility, thus offering a rare example of a transition-metal-free borylation protocol. Experimental and theoretical studies have been performed to elucidate the reaction mechanism, revealing the unusual formation of Lewis acid/base adduct between organohalides and α-borylcarbanion, generated in situ from the reaction of 1,1-bis[(pinacolato)boryl]alkanes with an alkoxide base, to facilitate the borylation reactions.


R1
X
(X = I, Br)
+
R2
pinB
Bpin
(R2 = H, Me)
NaOtBu
THF/toluene
50-120 °C
R1
Bpin
>35 examples
R1
Na⊕
X
R2
R1
Na⊕
Y−Bpin
Y = CH(R2)Bpin
or OtBu
• Transition-metal-free
• New type of borylation reagent
• Excellent C-B selectivity
• Broad substrate scope

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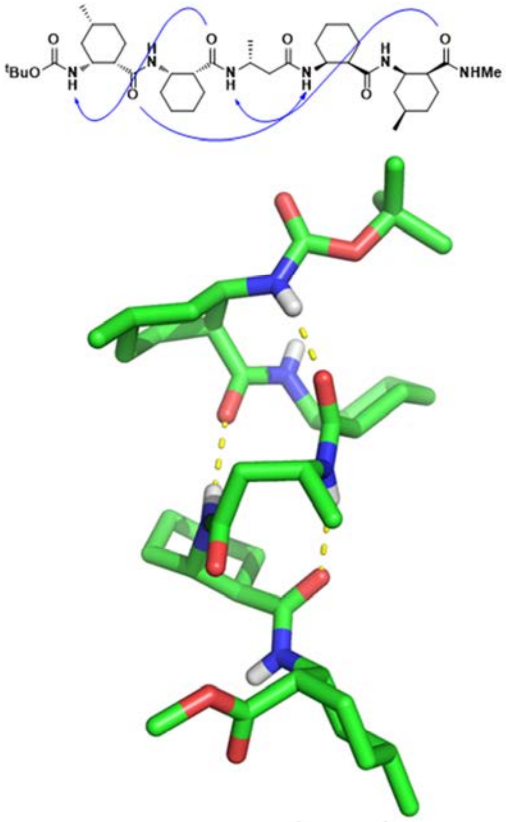
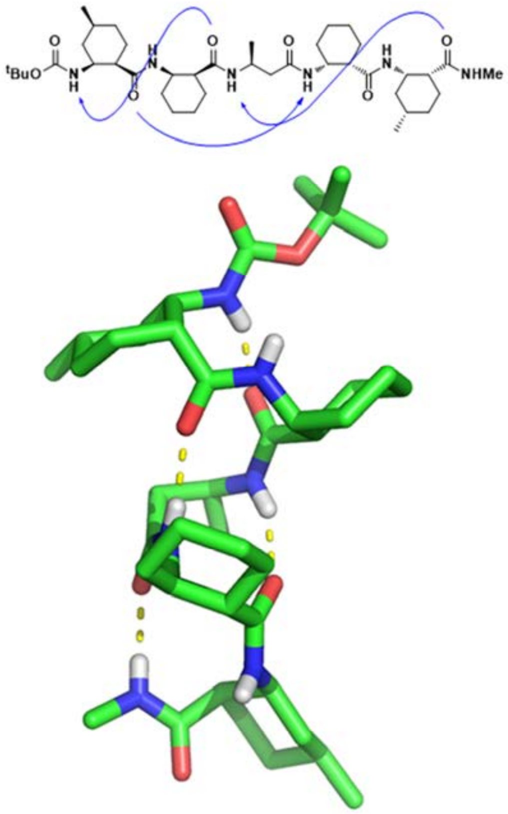
Dynamically Switchable 12/10-Helical β-Peptides Containing Malleable Acyclic β^3-Amino Acids

장근혁 최수혁*

연세대학교 화학과

Within the past two decades, the folding properties of several types of foldamers with unnatural backbones have been explored. Among them, β-peptides adopting well-defined secondary structures are particularly interesting as scaffolds. Herein we report that 12/10-helical propensity is well-maintained after partial replacement of cyclic β-amino acid residue with acyclic β^3-amino acid residue known to be quite malleable. In those 12/10-helices, unlike in earlier studies, acyclic L-β^3-residue has an unusual *gauche*(-) conformation in spite of steric strain, which is derived from high-resolution crystal structures. Our results show that acyclic β^3-amino acid residue can be successfully incorporated into the 12/10-helical β-peptide if most of the residues are appropriately pre-organized for folding, even though those β^3-residues have energetically unfavorable conformations. We hope that these results can enrich the domain of β-peptide foldamer chemistry.


^{t}BuO
NHMe


^{t}BuO
NHMe

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발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 박진규

Design of Enzyme-Active Probes and Their Application to Cancer Diagnosis

박석안 김해조*

한국외국어대학교 자연과학대학 화학과

In this presentation, I would like to discuss about the design of enzyme active probes and their application to tumor diagnosis in the mouse model of cancer, specifically by introducing a reactive group toward *g*−glutamyltranspeptidase (*g*GT).[1] As a cell surface-associated enzyme, *g*GT has been reported to be overexpressed in cervical, ovarin, and colon cancer. Especially colon cancer is difficult to detect in an early stage of the disease evolution and thus the diagnosis of colon cancer is an important issue. Herein, we report new activatable fluorescent probes from indocyanine that show selective and sensitive detection of tumor-enriched *g*GT. The probes exhibited a dramatic fluorescence enhancement (F/F_0 = 10) or ratiometric two wavelength emission upon the addition of *g*GT and then was applied for the successful detection of colon cancer in the mouse model.References: 1. Y. Urano, M. Sakabe, N. Kosaka, M. Ogawa, M. Mitsunaga, D. Asanuma, M. Kamiya, M. R. Young, T. Nagano, P. L. Choyke, H. Kobayashi, Sci. Transl. Med. 2011, 3, 110-119.2. S. Park, S.-Y. Lim, S. M. Bae, S.-Y. Kim, S.-J.Myung, H.-J. Kim, ACS Sens. 2016, 1, 579-583.3. S. Park, D. J. Bae, Y.-M. Ryu, S.-Y. Kim, S.-J.Myung, H.-J. Kim, Chem. Commun. 2016, 52, 10400-10402.4. S.-Y. Na, H.-J. Kim, Dyes Pigmen. 2016, 134, 526-530.

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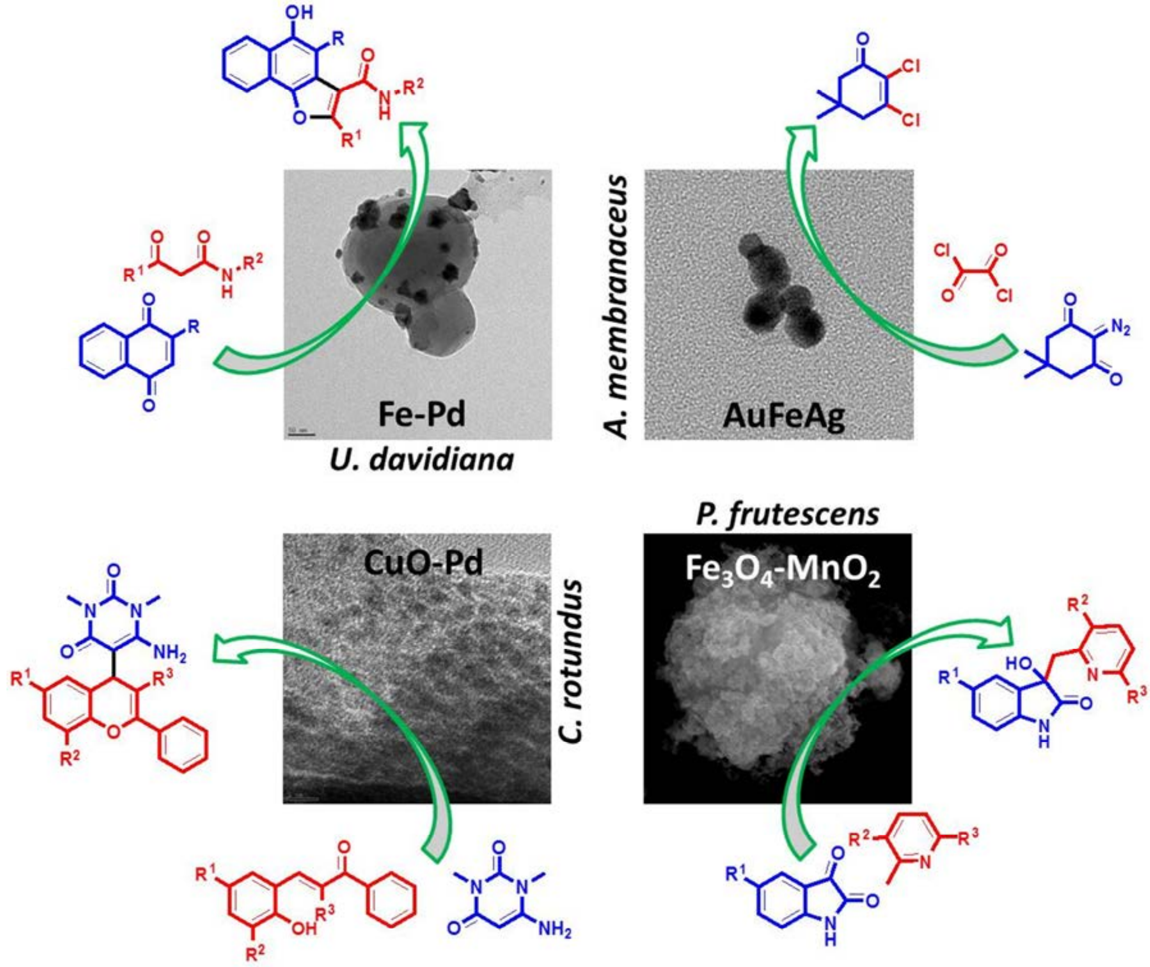
Metal and Metal Oxide Nanoparticles as an Efficient and Reusable Catalysts for the Organic Transformations

MISHRAKANCHAN 이용록*

영남대학교 화학공학부

Over the decades, metal and metal oxide nanoparticles (M-MO NPs) have attracted remarkable interest because of their significance in catalytic, magnetic and optical applications in a variety of fields. Despite the existing several physical and chemical synthetic routes, there is still a demand for better and eco-friendly approaches for the preparation of M-MO NPs. In this regard, we have successfully developed a rapid, non-toxic, and green protocol for the synthesis of M-MO NPs using plant extracts. As observed in many organic transformations, bimetallic transition metal based nanoparticles have shown higher catalytic activity than their monometallic counterparts. In this regard, we have synthesized bimetallic, trimetallic, and bimetallic oxide nanoparticles by green approach for catalytic activity. Herein, we present a facile and green approach for the synthesis of M-MO NPs using plant extract as reducing and capping agent. The synthesized M-MO NPs were applied as nanocatalysts for the organic transformations (Scheme 1). Moreover, the well characterized nanoparticles can be retrieved and reused for consecutive reactions without any significant loss in catalytic activity.



Scheme 1. Metal and metal oxide nanoparticles for the organic transformations.

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One-pot Synthesis of Quinolinones and Quinolinols through Cu-Catalyzed Aza-Michael Addition/Cyclization

강성일 이윤미*

광운대학교 화학과

2,3-Dihydro-4(1H)-quinolinones and 4-hydroxy-quinolines have been known to exhibit interesting biological properties such as BoNT/A LC inhibitors, analgesic and broad-spectrum antibiotic activity. Various methods have been developed, but there are some disadvantages to synthetic usability. For example, a long synthesis step is required and the reaction is carried out under harsh reaction conditions like high temperature and strong acid. Therefore, new synthetic approaches are still required. Inspired by our previous study involving Cu-catalyzed aza-Michael addition of anilines to phenyl vinyl sulfone to afford various β-amino sulfones with high efficiency, we developed an efficient and mild method for one-pot synthesis of 2,3-dihydro-4(1H)-quinolinone and 4-hydroxy-quinoline derivatives. One-pot synthesis is underwent via Cu-catalyzed aza-Michael addition of methyl 2-aminobenzoates to phenyl vinyl sulfones or vinyl ketones, followed by the treatment of in situ-generated β-amino groups with KOt-Bu to afford the cyclized products.

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Cube-in-cube nanoparticles for super-radiant photoluminescence

박정은* 남좌민*

서울대학교 화학부

Photostability of photoluminescence (PL) from metal nanostructures such as non-photoblinking and non-photobleaching is beneficial to exploit them as reliable optical probes. The localized surface plasmon of plasmonic nanostructures strongly interact and concentrate light in the nanoscale allowing high absorption cross-section, which can compensate relatively low quantum yield (QY). However, recent studies on PL from plasmonic nanostructures have mostly been limited to lithographically fabricated structures or simple nanoparticles such as nanospheres or nanorods. Here we designed and synthesized interior nanogap-engineered cube-in-cube (CiC) nanoparticles (NPs) in a high yield via a galvanic void formation process.1 The CiC shows significantly enhanced PL and the PL intensity and QY of CiC NPs are 31 times and 16 times higher than those of Au nanocubes, respectively, which have the highest PL intensity and QY reported for metallic nanostructures. We attribute the intense PL to super-radiant character of plasmon mode arisen from plasmonic coupling between the core and the shell. Finally, we check the long-term photostability of the PL signal under continuous illumination for 1 h.

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Nanospace-Confined Growth Behavior of Transition Metal Sulfides and Their Impacts on the Hydrogen Evolution Reaction

서보라 주상훈[1,*]

UNIST 화학과 [1]UNIST 에너지화학공학부

Two-dimensional layered transition metal dichalcogenides (2D TMDs) have been of tremendous recent interests as active electrocatalysts for the hydrogen evolution reaction (HER). Since TMD catalysts are commonly grown on conductive carbon supports, revealing their growth behavior on carbon surface can suggest rational design concept for the TMD-based HER catalysts. With an aim to investigate the growth orientation on carbon surface, we synthesized MS2 (M = W or Mo) nanoplates (NPs) within porous carbon nanorod arrays by limiting their growth space at the nanoscale. A combined experimental and computational study revealed that the horizontal growth is preferred in WS2 giving rise to monolayer NPs. In contrast, MoS2 NPs favor to adhere to the carbon surface in a vertical, edge-on bonding mode, which promotes subsequential stacking to generate multilayer NPs. In the space-confinement growth within carbon nanostructure, the monolayer WS2 grown along the curved surface of carbon nanorods may have highly strained surface sites affording a high density of active unsaturated S2- species. A series of monolayer WS2 NPs with different lateral sizes were prepared on carbon nanorods, and showed efficient HER activity with a high turnover frequency. A linear correlation between mass activities and ratios of S2-/S22- species is established, suggesting that active sites primarily originate from unsaturated S2- species in highly strained basal surfaces in monolayer WS2 NPs.

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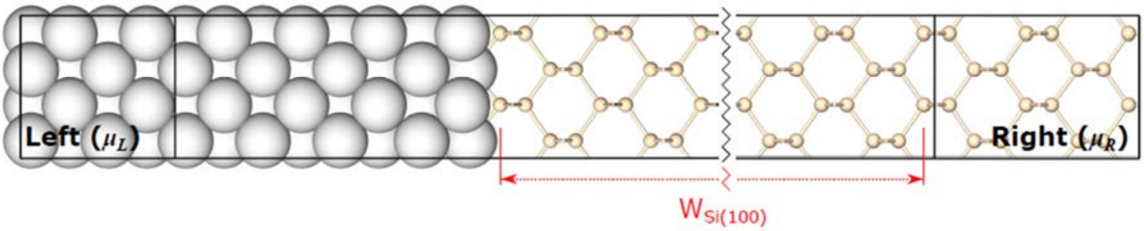
발표종류: 구두발표, 발표일시: 목 09:20, 좌장: 박영석

Atomic-scale modelling of interfaces in semiconductors and solar cell devices

이맹은 **Kurt Stokbro**[1,*]

QuantumWise 개발 [1]QuantumWise

As electronic devices shrink in size to reach nanoscale dimensions, interfaces between different materials become increasingly important in defining the device characteristics. In this talk I will present first principles calculations of the electrical properties of interfaces, based on Non Equilibrium Greens Function calculations (NEGF) using the ATK software. I will present calculations of the Schottky barrier at a Silicon-Silver interface, and calculate the dependence of the barrier on the doping and the applied bias. In another example, I will present calculations for the band offset between CZTS and CdS in a solar cell device and use the ab initio data in a multi-scale simulation of the solar cell efficiency.



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Free-standing, Two-dimensional Polymers and Their Applications

백강규[*] 김지홍[1] 김기문[1,*]

기초과학연구원 복잡계자기조립연구단 [1]POSTECH 화학과

Since the discovery of graphene, two-dimensional (2D) polymers have attracted significant attention for their great potential in electronics, selective transport, catalysis and chemical sensing. However, the lack of a robust method to produce such 2D conjugated polymers has hindered the investigation of both their fundamental aspects and wide practical applications. Recently, we developed a new approach to synthesis of free-standing 2D polymers by covalent stitching of disk-shaped building blocks in solutions or on substrates.[1,2] Depending on the intrinsic properties of the building blocks, these 2D polymers can be utilized as tailorable permselective membranes,[3] sensors, and resistive memory devices. Details of our recent discoveries and progress in covalent self-assembly of the 2D polymers will be discussed.References1. Baek, K.; Yun, G.; Kim, Y.; Kim, D.; Hota, R.; Hwang, I.; Xu, D.; Ko, Y. H.; Gu, G. H.; Suh, J. H.; Park, C. G.; Sung, B. J.; Kim, K. *J. Am. Chem. Soc.* **2013**, *135*, 6523-6528.2. Baek, K.; Hwang, I.; Roy, I.; Shetty, D.; Kim, K. *Acc. Chem. Res.* **2015**, *48*, 2221-2229.3. Baek, K.; Xu, D.; Murray, J.; Kim, S.; Kim, K. *Chem. Commun.* **2016**, *52*, 9676-9678.

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장소: 일산 KINTEX

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Synthesis of PdPtCu Dendritic alloy Nanoparticles and Their High Catalytic Performance with Methanol and Ethanol Oxidation

이영욱 한상우*

KAIST 화학과

The various applications of multi-metal nanocrystals were reported in fuel cell, organic catalysis, SERS and hydrogen storage materials application. Among others, PdPtCu alloy nanocrystal is important due to have different properties. Especially, tri-metal alloy nanoparticles (NPs) reported shape of sphere. However, we demonstrate that PdPtCu alloy dendritic nanoparticles (DNPs) could be exclusively prepared with generally controlled nanoparticles. Facile synthesis of PdPtCu alloy DNPs by using ascorbic acid as a reducing agent and cetyltrimethylammonium chloride (CTAC) as a capping agent is presented. The synthesized PdPtCu alloy DNPs were characterized by transmission electron microscopy (TEM), scannig electron microscopy (SEM), X-ray diffraction (XRD), and cyclic voltammetry (CV). The PdPtCu alloy NPs present efficient electrocatalysis with methanol oxidation (MOR) and ethanol oxidation (EOR).

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Hierarchically N-doped porous carbon nanofibers derived from crab shell: Application for CO2 adsorption and Metal oxide@Carbon supercapacitors

김희수 김동관 정희승 유원철*

한양대학교 응용화학과

Crab shell, a plentiful food waste and high volume organic resource, has been used to synthesize nitrogen and oxygen doped activated porous carbon. Crab shell (CS) that consists of chitin materials with CaCO3 and MgCO3 is changed to organic nanofibers using acid (HCl) treatment for removal CaCO3 and MgCO3. And these organic nanofibers were used to prepare micro- mesoporous crab shell derived carbon nanofibers (CSCNs) by a two-step carbonization, and subsequent CO2 activation process was performed to fine-tune specific surface area (SSA) and pore size distribution (PSD), denoted as CSCN_CXX, XX stands for the treatment time. The activated porous carbon shows high SSA of 2430 m2 g-1 and a large pore volume of 1.21 cm3 g-1 and high N-doping levels of 4.6 wt%.As a CO2 adsorbent, the porous carbon has good CO2 adsorption capacities (6.09 mmol g-1 at 273K and 3.72 mmol g-1 at 298K under 1bar) and a good CO2/N2 selectivity (33.6@298K), which is calculated from the single-component adsorption isotherms based on the ideal adsorption solution theory (IAST) method. As an electrode material, the porous carbon exhibits good electrochemial 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 (80%) for over 10000 cycles (current density at 2 Ag-1) . In addition, highly N-doped hierarchical CSNCs are used as hybrid supercapacitors decorated with Fe2O3 and CO3O4 metal oxide nanoparticles (Fe2O3@CSCN, Co3O4@CSCN). Fe2O3@CSCN and Co3O4@CSCN composites show outstanding capacitances of 291 Fg-1 and 508 Fg-1 at 1 Ag-1, excellent retention of 183 Fg-1 (63%) and 374 Fg-1 (74%) at 50 Ag-1. And these hybrid materials also show outstanding long-term cycling stabilities of 253 Fg-1 (91%) and 470 Fg-1 (95%) at 2 Ag-1 over 10000 cycles. This works shows a good instance for taking advantage of recycling food garbage and proving applications in energy storage materials and CO2 gas sorbents.

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Facile Surface Tailoring of Reduced Graphene Oxide Using Capping Agents for Nonmetallic Catalysis

송재은 한상우*

KAIST 화학과

Reduced graphene oxide (rGO) functionalized with organic capping agents has gained increasing attention as a promising metal-free catalyst. To optimize the properties of rGO for target applications, comprehending the link between the catalytic function of rGO and the chemical and structural characteristics of capping agents is critical. Herein, we report a systematic study on the effect of capping agents on the catalytic function of rGO for redox reactions using nitrogen-containing surface modifiers with distinctly different chemical structures, such as poly(diallyldimethylammonium chloride), cetyltrimethylammonium chloride, and poly(allylamine hydrochloride), which have the capability to endow rGO with improved suspension stability, enhanced reactant adsorption, and modified electronic properties. Functionalized rGOs were facilely prepared by the reduction of graphene oxide with hydrazine in the presence of the capping agents. The results of model redox reactions, i.e., 4-nitrophenol and ferricyanide reduction reactions, catalyzed by the functionalized rGOs corroborated that the way the capping agents functionalize rGO, which is highly correlated with their chemical structure, drastically influences the overall reaction kinetics, including induction time, reduction rate, total reaction time, and reaction order. This strongly suggests that the judicious selection of capping agents is crucial to fully harness the catalytic function of rGO and thus to design novel rGO-based non-metallic catalysts with controllable reaction kinetics.


Capping Agent-Functionalized rGO
Pseudo 0th order
Pseudo 1st order
NO2
OH
Bare
PDDA
CTAC
PAA
NH2
OH
FINISH

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발표종류: 구두발표, 발표일시: 목 10:10, 좌장: 박진균

Effect of atomic substitution and doping on thermoelectric properties of polycrystalline SnSe material

이용규 정인*

서울대학교 화학생물공학부

Thermoelectric power generation is in the focus of considerable attention because of the potential for environmentally benign and cost-effective conversion of waste heat to electricity. A single crystalline form of p-type SnSe has recently shown an exceptionally high ZT of ~2.6 at 923 K along the b-axis due to a highly anharmonic bonding. Since then polycrystalline SnSe based materials have been quite actively investigated for practical applications. However, it is quite difficult to make a high ZT polycrystalline SnSe material because of both low dopability and solubility limit with other elements. Thus, we investigated the effects of atomic substitution and doping on the thermoelectric properties of polycrystalline SnSe materials. In this study, we present detailed investigations of electrical and thermal transport measurement as well as structural data on polycrystalline SnSe based materials. Their thermoelectric properties are highly enhanced and its origin will be discussed.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT.O-9**

발표분야: Oral Presentation of Young Material Chemists

발표종류: 구두발표, 발표일시: 목 10:20, 좌장: 박진균

Injectable hydrogels derived from alginate-alendronate calcium complexes for bone regeneration

김한샘 신원상[1,*]

단국대학교 나노바이오의과학과 [1]단국대학교 나노바이오의과학

Modification of sodium alginate was conducted by the functionalization of alginate with Alendronate and calcium complex formation using $Ca(OAc)_2$ finally to get alginate-alendronate calcium complexes (Alg-Alen/Ca) containing calcium and phosphate ions. The obtained alginate derivatives including Alginate-Alendronate (Alg-Alen) and Alginate-Alendronate calcium complex (Alg-Alen/Ca) were characterized by Fourier transform infrared spectroscopy, nuclear magnetic resonance spectroscopy for ^1H nuclei, high resolution inductively coupled plasma optical emission spectroscopy, and thermogravimetric analysis. The new injectable hydrogels (Alg-Alen/Ca/Alg) were simply prepared by mixing Alg-AlenCa solution with NaAlg solution in different volume ratios (40:60, 50:50, 60:40) without additional calcium salt supply externally. The gelation was completed within 5-15min indicating a high potential of hydrogel delivery by injection to in vivo. SEM analysis of the prepared injectable Alg-Alen/Ca/Alg hydrogels showed highly porous morphology with interconnected pores of width in the range of 180-630μm. In vitro 3D cell study using mesenchymal stem cell showed that the injectable hydrogels exhibited comparable properties to the cell culture plate in terms of cytotoxicity and differentiation of MSCs. The developed injectable hydrogels showed a high degree of biocompatibility and significantly higher ALP gene and ARS expressions, suggesting the potential application in bone tissue engineering and regenerative medicine.

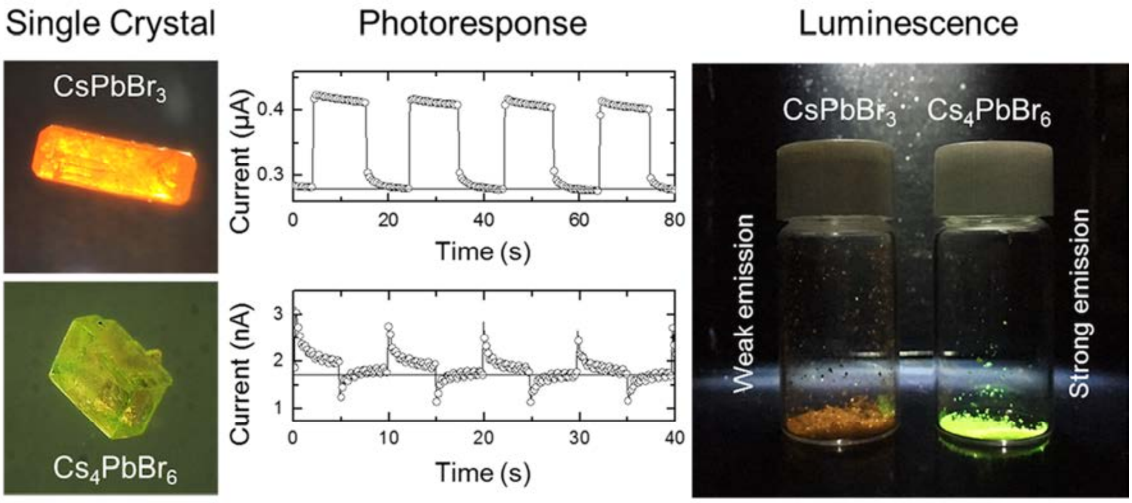
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.O-10**
발표분야: Oral Presentation of Young Material Chemists
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 박진균

Correlation Between Photoreresponse and Crystal Structure of Cesium Lead Bromide Perovskites

차지현 박용민 박철우[1] 안태규[1] 정덕영[*]

성균관대학교 화학과 [1]성균관대학교 에너지과학과

The analogues of cesium lead bromide promise outstanding optical and electrical properties, significantly more stable than organic-inorganic hybrid perovskite in ambient atmosphere. Pure $CsPbBr_3$ and Cs_4PbBr_6 single crystals were separately grown by AVC (anti-solvent vapor-assisted crystallization process) with dimensions of millimeters. We found the correlation between photocurrent generation and PL (photoluminescence) in perovskite crystals. The $CsPbBr_3$ crystals, which have 3D perovskite structure, showed a sensitive steady-state photoresponse and a poor PL signal. Contrastively, the Cs_4PbBr_6 crystals, which have 0D perovskite structure, exhibited more than 1 order magnitude higher PL intensity than $CsPbBr_3$, which generated an ultralow photocurrent under illumination. We attribute their contrasting opto-electrical characteristics to a difference of exciton binding energy, induced by coordination geometry of $[PbBr_6]^{4-}$ octahedron sublattice. Our works help to wide the understanding of the relation of chemical structure with PL and photocurrent generation of perovskite compounds.


Single Crystal
Photoresponse
Luminescence
CsPbBr3
Cs4PbBr6
Current (μA)
0.4
0.3
0 20 40 60 80
Time (s)
Current (nA)
3
2
1
0 10 20 30 40
Time (s)
CsPbBr3
Cs4PbBr6
Weak emission
Strong emission

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT.O-11**

발표분야: Oral Presentation of Young Material Chemists

발표종류: 구두발표, 발표일시: 목 10:40, 좌장: 박진균

Tailoring the size of Au nanoparticle clusters through sacrificial template assembly method for investigation of size effects in optimal SERS performance

이승훈 한상우*

KAIST 화학과

The assembly nanostructures offer many advantages for enhanced plasmonic performance through a precise control over both the gap size and the particle size. Although the many assembly strategies have been reported in colloidal solution, there are some issues with structural stability and facile synthesis method due to their assembly forces sensitive to environmental stimuli. Here, we manipulate the size of constituent particle in nanoparticle clusters (NPCs) easily through a sacrificial template mediated assembly strategy. Due to the intrinsic assembly force of our assembly strategy such as Van der Waals force and capping agent interaction, the prepared Au NPCs demonstrate remarkable structural stability and SERS performance even in harsh conditions such as strong acidic (pH 2) or basic (pH 12) condition. Furthermore, the new tendency of size effect in SERS is observed that the smaller particle size demonstrates the strong SERS performance than the larger particle size in well-defined assembly structures. Finite-difference time-domain (FDTD) calculations support our results through induction of the competition between the intensity of hot spot and the area of hot spot.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT.O-12**

발표분야: Oral Presentation of Young Material Chemists

발표종류: 구두발표, 발표일시: 목 10:50, 좌장: 박진균

Multiplexed detection strategy using optokinetically encoded nanoparticles on lipid bilayer

김선기 남좌민*

서울대학교 화학부

Multiplexed real-time analysis on multiple interacting molecules and particles is needed to obtain valuable information in a complex medium, often found in chemical and biological systems. In particular, multiplexed profiling of microRNA (miRNA) in a reliable, quantitative manner is of great demand for the use of miRNA in cell biology, biosensing and clinical diagnostic applications. Here, we report a multiplexed miRNA detection strategy using optokinetically (OK) coded nanoprobes (NPs) that show distinct optical signals and dynamic behaviors on a supported lipid bilayer (SLB) (OK-NLB assay).[1] Metal NPs with three distinct dark-field light scattering signals [red (R), green (G) and blue (B)] and three different target miRNA half-complements were tethered to two dimensionally fluid SLB with mobile (M) or immobile (I) state. In situ single-particle monitoring and normalized RGB analysis of the optokinetically combinatorial assemblies between three M-NPs and three I-NPs with dark-field microscopy (DFM) allow for differentiating and quantifying 9 different miRNA targets in one sample. The OK-NP-based assay enables simultaneous detection of multiple miRNA targets in a highly quantitative, specific manner within 1 hour, and can be potentially used for diagnosis of different cancer types.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.O-1**
발표분야: Oral Presentation of Young Scholars in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 이재준

Electrocatalytic Hydrogen Production on Atomically Precise $M@Au_{24}(SR)_{18}$ (M=Au,Pt) Nanoclusters

최우준 이동일*

연세대학교 화학과

Atomically precise gold nanoclusters containing from a few to a few hundreds of atoms have received great attention due to their unique electronic structure, stability and catalytic activity. Especially, ultrasmall Au_{25} nanocluster that contains 25 Au atoms has distinctive catalytic activity for renewable energy production such as CO_2 reduction reaction (CO_2 RR) and hydrogen evolution reaction (HER). Furthermore, the activity and selectivity for the catalytic reactions can be easily modified by introducing the foreign metals such as Pt and Pd in Au_{25} platform. In this presentation, we successfully synthesized the ultrasmall Au nanocluster, $Au_{25}(SR)_{18}$ (SR=thiolate), and bimetallic clusters $MAu_{24}(SR)_{18}$ (M=Pt) and revealed their electronic structures and catalytic properties. Au_{25} have remarkable catalytic activity for CO_2 RR with high selectivity for CO over H_2 at low overpotential where it has poor activity for HER. Enhanced catalytic activity for HER was observed by doping of a Pt atom into Au_{25} nanocluster. Pt doped nanocluster, $PtAu_{24}$, have very low onsetpotential (E_{onset} = 70mV vs. RHE) that is comparable to that of natural hydrogenase (~100 mV) enzymes and high TOF value that is 34 mol H_2 mol/cat·s (at $\eta = 0.6$ V) for electrocatalytic HER owing to decreased reduction potential and thermodynamically neutral binding energy of proton on Pt atom. These modified catalytic activities of Au_{25} and $PtAu_{24}$ suggests that doping of clusters is a powerful means to fine-tune the catalytic properties of clusters, offering special advantages in the development of new functional electrocatalysts.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.O-2**
발표분야: Oral Presentation of Young Scholars in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 이재준

Electrochemical CO_2 conversion in aqueous solution via Metal Cluster

이용진 이동일*

연세대학교 화학과

Much effort has been made to convert carbon dioxide into a useful substance to prevent the greenhouse effect of carbon dioxide, a by-product of fossil fuels. However, the conversion of carbon dioxide requires a lot of energy input, so it is important to develop suitable catalysts, and catalysts using metal are being actively developed. Our group used a metal cluster consisting of 25 gold atoms as a catalyst, and improved catalyst selectivity and reactivity in the conversion of carbon dioxide. In this experiment, a glassy carbon electrode carrying gold nanoclusters was used as an electrode for electrochemical conversion, and carbon dioxide was converted into carbon monoxide and hydrogen on an aqueous solution(pH 7), which was analyzed using a gas chromatographic system. Faradaic efficiency was observed at 90% (overvoltage : 0.4 V) and J_{co}(Partial Current) value was 13 mA/cm2(overvoltage : 0.6 V). In the same method, the conversion experiment of carbon dioxide was carried out using Au_{25} based $PtAu_{24}$. Compared with Au_{25}, single Pt atom doped $PtAu_{24}$ are selective for H_2. The study described here has more significance towards the understanding of CO_2 reduction reaction on metal nanoclusters and their alloys.

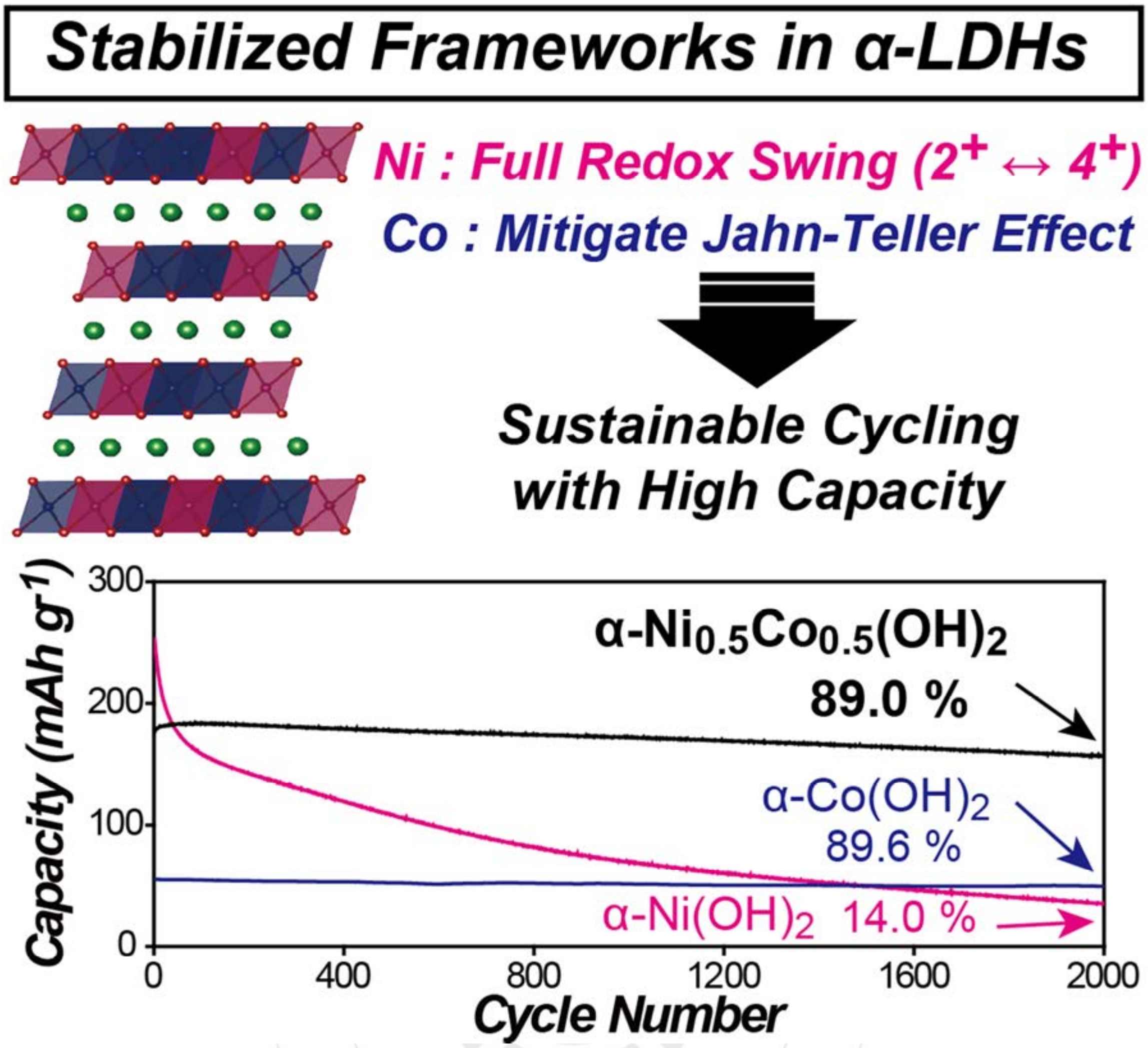
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.O-3**
발표분야: Oral Presentation of Young Scholars in Electrochemistry
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 이재준

Stabilized Octahedral Frameworks in Layered Double Hydroxides by Solid-Solution Mixing of Transition Metals

이지훈 최장욱*

KAIST EEWS

Pseudocapacitors have received considerable attention, as they possess advantages of both rechargeable batteries and electric double layer capacitors. Among various active materials for pseudocapacitors, α-layered double hydroxides (α-TM(OH)2, TM = transition metal) are promising due to their high specific capacities. Yet, irreversible α-to-β phase transitions of α-TM(OH)2 hinder their long-term cyclability, particularly when the TM is nickel. Here, it is reported that binary TM ion mixing can overcome the limited cycle lives of α-TM(OH)2 by stabilizing the octahedral frameworks of α-TM(OH)2. In particular, an α-TM(OH)2 with equal amounts of nickel and cobalt exhibits long-term capacity retention (89.0% after 2000 cycles) and specific capacity (206 mAh/g), which are better than those of individual TM counterparts. A series of analyses reveals that the improved performances originate from the synergistic effects between the TM ions; the preferred trivalent state of cobalt ions stabilizes the octahedral framework by accommodating the detrimental Jahn–Teller distortion of Ni3+. The stabilized framework also widens the redox swing range of the nickel up to 4+, thus, increasing the specific capacity of the corresponding α-TM(OH)2. This study indicates that proper mixing of TMs is a prolific approach in enhancing the vital properties of α-TM(OH)2, a promising family of pseudocapacitor materials.Keywords: Layered Double Hydroxide, Electrochemistry, X-ray Absorption Fine Structure Analysis, Crystal Field Theory(Ref) Ji Hoon Lee et al., Adv. Funct. Mater., 2017, DOI:10.1002/adfm.201605225)


Stabilized Frameworks in α-LDHs
Ni : Full Redox Swing (2+ ↔ 4+)
Co : Mitigate Jahn-Teller Effect
Sustainable Cycling with High Capacity
Capacity (mAh g-1)
300
200
100
0
0
400
800
1200
1600
2000
Cycle Number
α-Ni0.5Co0.5(OH)2
89.0 %
α-Co(OH)2
89.6 %
α-Ni(OH)2 14.0 %

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC.O-4**

발표분야: Oral Presentation of Young Scholars in Electrochemistry

발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 이재준

Graphene-wrapped Porous Sb Anodes for Rechargeable Sodium-Ion Batteries by Mechanochemical Compositing and Metallomechanical Reduction of Sb_2O_3

황치현* 양주찬

UNIST 에너지공학과

Antimony metal nanoparticles wrapped with a-few-layer graphene coat (Sb@Gn) were prepared from their oxide form (Sb_2O_3) in a micrometer dimension by a novel two-step ball-milling process. The first mechanochemical process was designed to decrease the particle size of Sb_2O_3 microparticles for advantage of nano size and then coat the Sb_2O_3 nanoparticles with a-few-layer graphene (Sb_2O_3@Gn). The second metallomechanical ball milling process reduced the oxide to its metal form (Sb@Gn) by the help of Zn as a metallic reductant. The graphene layer (@Gn) blocked the alloying reaction between Sb and Zn and limited the size of Sb particles during the metallomechanical reduction step. The redox reaction of Sb_2O_3@Gn was presented via oxygen direct transfer and the redox transfer though two type vacancies in graphene layer. The Sb@Gn anode showed outstanding capacity retention along cycles and improved rate capability in sodium ion batteries. The @Gn played roles of providing conductive pathways to Sb core and limiting the size expansion during sodium alloying step.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC.O-5**

발표분야: Oral Presentation of Young Scholars in Electrochemistry

발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 이재준

Stand-alone carbon dioxide reduction using copper oxide wire arrays powered by WO3/DSSC dual absorbers

<u>최승요</u> 박현웅[1,*]

경북대학교 건설환경에너지공학부 [1]경북대학교 에너지공학부

We have developed a tandem photoelectrochemical cell which is composed of WO_3/dye-sensitized TiO_2 (WO_3/dye) dual absober photoandoe and copper oxide (Cu_2O/CuO) wire array cathode. This tandem cell is demonstrated as a stand-alone and durable device for CO_2 photoelectrochemical reduction. The Cu_2O/CuO wire arrays exhibits a superior electrocatalytic activity of CO_2 reduction compared to metallic Cu (Cu0). Upon irradiation of a simulated light (AM 1.5; 100 mW/cm2), the single absorber system (WO_3 and Cu_2O/CuO couples) shows low open circuit potential at -0.2 V (0.1 M potassium bicarbonate; pH 6.8; carbon dioxide-purged). In the dual absorber system, the long wavelength (> 450 nm) passed through the semi-transparent WO_3 film is absorbed by dye. The tandem PEC cell shows open circuit potential gain of ~0.7 V, which can drive the CO_2 conversion without any external bias. The primary CO_2 conversion product is CO with energy efficiency ~3.5 % while H_2 and low amount of formic acid are obtained with the energy efficiencies of ~0.9 % and ~0.35 % in 5 hours, respectively. The significant low yield of formic acid is attributed to the limited availability of proton/electron pairs (H•) at less negative potentials leading to predominant CO formation, as well as at high negative potentials due to predominant H_2 production. Neither CO_2 conversion products nor H_2 are not found in the single absorber system

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC.O-6**

발표분야: Oral Presentation of Young Scholars in Electrochemistry

발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 이재준

Development of photo-assisted microbial electrolysis cells for the persistent hydrogen production

전용원 김성현[1,*]

건국대학교 생명공학과 [1]건국대학교 특성화학부생명공학과

A microbial electrolysis cell (MEC) is a device that converts organic matters to hydrogen with an additional external voltage input. Protons and electrons produced by microbes at the anode are transferred to the cathode and combined to molecular hydrogen. Since the hydrogen gas can be produced without a fermentation barrier and in an environmentally friendly way, an MEC has been regarded as an alternative to the conventional methods. Here we show that photo-assisted MECs could be developed using p-type semiconductors such as polyaniline nanofiber (PANInf) and CuO as cathodes under visible light illumination. We found that under 0.8 V external bias and light illumination in a single-chamber MEC, continuous hydrogen production from acetate were achieved at a rate of 1.78 and 1.84 m^3 H_2/m^3d with negligible methane formation with PANInf and CuO, respectively. These values are favorably compared with that of Pt/C cathode that gives a rate of 2.17 m^3 H_2/m^3d. These results are attributed to the p-type semiconductor characteristics of the materials where photoexcited electrons are used to reduce protons to hydrogen at the cathode surface and holes generated in the valence band are filled with electrons from acetate oxidation at the anode. This work can be extended to the microbial wastewater treatment for the hydrogen production.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.O-7**
발표분야: Oral Presentation of Young Scholars in Electrochemistry
발표종류: 구두발표, 발표일시: 목 10:30, 좌장: 이재준

Electrochemiluminescence of Water-soluble Poly(amidoamine) Dendrimers Conjugated with Multiple Ru(II) Tris(bipyridine) Moieties

이혜인 김주훈*

경희대학교 화학과

We reported intense electrochemiluminescence (ECL) of water-soluble $[Ru(bpy)_3]^{2+}{}_n$–dendrimer (n = 7.5) conjugates which are tris(bipyridine)ruthenium(II) ($[Ru(bpy)_3]^{2+}$, where bpy = 2,2’-bipyridine)-functionalized poly(amidoamine) (PAMAM) dendrimers in the absence of any additional coreactant. $[Ru(bpy)_3]^{2+}$ was covalently conjugated to PAMAM dendrimers *via* reaction of $[Ru(bpy)_3]^{2+}$–NHS esters with terminal primary amines of dendrimers. We demonstrated the coreactant effect of Gn-NH_2 (n = 2, 4, and 6) dendrimers for the ECL of $[Ru(bpy)_3]^{2+}$ where $[Ru(bpy)_3]^{2+}$/G4-NH_2 system exhibited the largest ECL emission, which is ~23 times larger than that obtained in the absence of the dendrimers. It was also found that interior tertiary amine moieties of the dendrimer are primarily responsible for the coreactant effect of Gn-NH_2 (n = 2, 4, and 6) dendrimers. Based on the considerable coreactant effect of G4-NH_2 dendrimers, we synthesized $[Ru(bpy)_3]^{2+}{}_n$–G4-NH_2 dendrimer (n = 7.5) conjugates. The resulting water-soluble dendritic conjugates exhibited ~9-fold enhanced ECL intensity compared to ECL obtained from corresponding aqueous mixtures, including the same amounts of free G4-NH_2 dendrimers and $[Ru(bpy)_3]^{2+}$ complexes.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.O-1**
발표분야: New Trends in Chemistry Education
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 강석진

초등 과학 교과서에서의 인포그래픽스의 유형과 특징: 화학 영역을 중심으로

임희준

경인교육대학교 과학교육과

교과서는 시각적 자료와 텍스트를 통하여 내용을 전달한다. 기존에는 시각적 자료가 그림, 사진, 만화, 도표 등의 삽화로 텍스트가 제공하는 정보를 보완하거나 보충하는 형태이며, 텍스트와는 분리되는 그래픽의 형태가 많았다. 따라서 삽화 연구도 이러한 그래픽 유형의 측면에서 주로 이루어졌다. 그러나 최근에는 그래픽과 정보를 융합한 인포그래픽이 정보를 보다 효과적으로 전달하는 방법으로 활용되고 있다. 이에 초등과학 교과서에서 화학 영역에 사용되는 시각적 자료를 단순한 일밚 삽화와 인포그래픽으로 구분하고, 각각의 유형과 역할, 특징 등을 살펴보았다. 이를 통해 화학 영역에서의 시각적 자료의 특징을 고찰해보고자 하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.O-2**
발표분야: New Trends in Chemistry Education
발표종류: 구두발표, 발표일시: 목 09:25, 좌장: 강석진

돌턴의 사고를 적용한 수업에서 학생의 대기에 대한 개념변화

백성혜

한국교원대학교 화학교육과

돌턴의 입자에 대한 생각은 자연 현상(특히, 대기)을 이해하는데 매우 중요하다. 그러나 입자마다 질량이 다르기 때문에 중력의 영향이 다르다는 돌턴의 생각은 대기가 균질하다는 개념과 충돌한다. 대부분의 과학교과서는 대기를 균질한 질량으로 기술하고 있다. 균일한 공기 질량으로부터 다양한 질량 입자의 덩어리라는 개념변화는 현대과학의 관점에서 자연현상을 이해하는데 중요하다. 따라서 본 연구는 돌턴의 이러한 사고를 적용한 수업이 학생의 대기에 대한 개념변화에 어떠한 영향을 미치는지를 알아보았다. 8 학년 학생(N=146)과 11 학년 학생(N=90)를 대상으로 교실 안, 5km 까지의 대기, 1000km 까지의 대기의 연직 분포에 대한 생각을 조사하였다. 이후 돌턴의 입자에 대한 생각과 이에 따른 질량이 다른 입자의 중력 차이를 알아보는 수업활동을 전개하였다. 수업 후, 동일한 사후검사를 실시한 결과 학생들은 바라보는 대기의 규모에 따라 대기의 연직분포에 대한 생각이 과학적 개념으로 변화하였다. 이는 현재 교과서나 교육과정에서는 대기에 대한 부분을 다룰 때, 당연히 입자가 있다는 연역적 입장을 도입한다. 하지만 돌턴의 사고를 도입한 귀추적 사고는 학생들을 과학적 개념으로 도달하게 하는데 과학교육의 시사점이 있다고 할 수 있다. 따라서 화학에서 입자론이 도입되는 중학교 교육과정에 돌턴의 사고를 통한 귀추적 사고를 학생들이 경험할 수 있도록 돌턴의 창의적 사고를 교육과정에 반영할 것을 제안한다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.O-3**
발표분야: New Trends in Chemistry Education
발표종류: 구두발표, 발표일시: 목 10:10, 좌장: 강석진

사회-과학적 이슈 수업에서 나타난 학생과 교사의 딜레마

박현주

조선대학교 과학교육학부

현대 사회에서 발생하는 많은 과학과 관련된 논쟁들은 '과학'사용의 중요성과 유용함, 신중함을 깨닫게 한다. 또한 이것은 과학교육이 인간과 사회와의 상호협력적인 관계 속에서 이루어져야 한다는 것을 의미한다. 사회-과학적 이슈(Socio-Scientific Issue, SSI) 교육은 그동안 과학교육에서 '과학적' 접근으로 인하여 상대적으로 소홀했던 공동체 의식, 인성, 감성 등의 인간적, 윤리적, 자연애적인 측면 등을 강조한다. SSI 교육은 윤리적, 사회적, 도덕적 발달, 감성적 추론과 인성교육, 공동체 의식, 시민 의식 등을 동반한 '확장된' 과학적 소양의 함양을 추구한다. SSI 를 통해 과학기술 사회 및 학습에 대해 관심과 흥미를 유발하고, 개인의 과학적 소양 및 이공계 전문가의 올바른 윤리(가치관)의 함양을 목표로 한다. 본 연구에서는 중학생 학생들의 SSI 선호 주제를 조사하고, SSI 수업에서 나타난 학생과 교사의 딜레마를 조사하였다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **EDU.O-4**

발표분야: New Trends in Chemistry Education

발표종류: 구두발표, 발표일시: 목 10:35, 좌장: 강석진

과학교육을 통한 인성역량 함양

남정희

부산대학교 화학교육과

인성교육의 필요성은 전 세계적으로 이루어지고 있는 교육개혁이 표방하는 지향점중 하나인 21 세기를 살아가기 위한 미래시민으로서 갖추어야할 핵심역량중 하나이다. 인성교육은 그 동안 교육현장에서 여러 가지 형태와 방법으로 이루어져 왔으나 실제적으로 인성프로그램이 큰 효과를 거두지 못한 근본적인 이유 중 하나는 인성교육이 현재 학교교육의 맥락과 동떨어져 있으며 학생에게도 유의미한 경험을 제공하기 어렵다는 점이다. 또한 대부분 인성교육에 대한 일반적 방법 및 비교과 영역에서의 인성교육 모델에 대한 제안으로 그치고 있어 학교 수준에서 인성교육이 실행되는데 어려움이 있다. 따라서 학교 수준에서의 인성교육이 실행되기 위해서는 교과수준에서의 구체적인 인성교육 실천 방안이 필요하다. 그러나 아직까지는 교과수준에서 인성교육 방법에 대해서는 논의가 부족한 실정이며, 특히 과학교과에서 구체적인 인성교육 방안과 교수학습모델에 대한 논의는 부족한 실정이다. 과학이 다른 학문과 구별되는 특징적인 요소로는 탐구과정을 들 수 있다. 과학은 탐구과정에 근거를 두고 있으며, 탐구는 단순히 실험활동을 통한 지식의 습득과정이 아니라 과학자들의 과학적 의사소통의 과정이며 문제해결의 과정이다. 과학은 추론과 논의를 통한 점진적이고 합리적인 합의에 의해 발전하는 학문이다. 이런 점에서 과학의 탐구과정은 위에서 언급한 핵심역량이 실제 상황에서 길러질 수 있는 기반을 제공할 수 있다. 이러한 과학이라는 학문의 본성은 과학이 인성교육을 실행하기에 적합한 교과라는 것을 보여준다. 따라서 ‘과학교과’는 학생들의 인성을 함양할 수 있는 ‘도구’이자 ‘목적’으로 이용할 수 있을 것이다. 최근 연구자들 사이에서 과학 교육 분야에서도 인성교육과의 통합적 접근을 강조해야한다는 주장들이 제기되고 있다. 따라서 범교과적인 인성교육과 독립된 형태로 과학교과 내에서 인성교육에 관한 연구가 이루어져야 할 시점이다. 이에 따라 인성 교육에

대한 연구가 미비한 과학교과에서 바른 인성 함양을 목표로 하는 인성교육을 통합한 과학교육을 할 수 있는 방안이 마련되어야 할 것이다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.O-7**
발표분야: Current Trends in Environmental and Energy Chemistry
발표종류: 분과기념강연, 발표일시: 목 10:35, 좌장: 김동욱

Solar Conversions at the Interface of Semiconductor Hybrids for Energy and Environmental Applications

최원용

POSTECH 환경공학부

The photoinduced electron transfers occurring at the semiconductor interfaces are the key step of solar-driven photosynthetic and photocatalytic processes that are frequently investigated for their environmental significance. Metal oxides such as TiO2, WO3, and Fe2O3 that consists of earth-abundant elements are the most practical base materials for such applications. Despite their popularity as solar conversion materials, breakthroughs in materials development have yet to be achieved for practical applications. A variety of approaches have been investigated to modify the base metal oxides using diverse inorganic and organic materials. The heterojunctions built at the interface of semiconductors reduce the charge recombination or enhance the interfacial charge transfer to achieve the higher conversion efficiency. In this talk, various modifications of metal oxides with interfacial heterojunctions will be introduced and discussed for photoelectrochemical and photocatalytic conversions for environmental applications. The specific examples include dual-purpose photocatalysis for H2-recovering water treatment, barrier layer passivation on the semiconductor surface for enhancing photoconversion efficiencies, TiO2/graphene composites, titania nanotubes for the photocatalytic removal of volatile organic compounds, charge transfer complexation on the surface of TiO2, and carbon nitrides as an environmental photocatalyst.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.O-1**
발표분야: Current Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:00, 좌장: 한승희

Membrane toxicity of polyhexamethylene guanidine(PHMG) as a humidifier disinfectant

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POSTECH 환경공학부 [1]POSTECH 환경대학원

Many pollutants, toxins, antibiotics or antimicrobial compounds interact against biological membranes, and precise evaluation on the molecular interaction between biological membrane and the potentially toxic chemical is essential to foresee the toxicity and bioavailability of newly synthesized molecules. In this study, a surface forces apparatus (SFA) measurement and Langmuir trough based tensiometry are combined to reveal molecular interaction mechanisms between potentially toxic compounds and biological membranes for toxicity evaluation. As a toxic compound, polyhexamethylene guanidine (PHMG), was selected because humidifier disinfectant and Vodka containing PHMG caused a lot of victims in both S. Korea and Russia, respectively, due to the lack of holistic evaluation on the toxicity of PHMG. We measured strong adhesion (Wad~4.2 mJ/m^2) between PHMG and the lipid membranes, and a significant change in π-A isotherm of DPPC monolayers upon PHMG adsorption. These results indicate that PHMG strongly binds to hydrophilic head group of lipid membrane and alter the structural and phase behavior of lipid membranes. Overall, combining SFA and Langmuir trough techniques are useful to predict the potential toxicity of a chemical by evaluating the molecular interaction with biological membranes, the primary protective barrier for living creatures.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.O-2**
발표분야: Current Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:15, 좌장: 한승희

Formation of diverse Mn oxides by various geochemical reactions

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연세대학교 지구시스템과학과

Mn (oxyhydr)oxides (collectively referred to as oxides) are widely distributed in the environment (e.g., soil, groundwater, ocean, and hydrothermal vent) and playing an essential role together with Fe oxides by controlling the fate and transport of various chemical species (e.g., nutrients, contaminants). A variety of Mn oxides have their unique physico-chemical properties and reactivity, which are correlated to the different atomic arrangement, wide ranging of crystallinity, and mixed valence of structural Mn. Previous studies have mostly focused on the mobility of various contaminants by the sorption and redox reactions with specific Mn oxides. However, the geochemical processes of diverse Mn oxides formation under varying environmental conditions have not been fully understood yet. Hence, this study aimed at investigation of the geochemical factors controlling the formation and phase transformation of diverse Mn oxides through various redox reactions.

Batch experiments were conducted through homogeneous or surface catalyzed Mn(II) oxidation, and during the redox reactions of Mn oxides (i.e., birnessite) with aqueous Mn(II) or common redox sensitive materials (i.e., $Cr(OH)_3$(s)). The results of homogeneous Mn(II) oxidation ($[Mn(II)]_0$ = 0.05 or 1.0 mM) at pH 9.0 open to the atmosphere showed the production of pure hausmannite (Mn_3O_4), whereas surface catalyzed Mn(II) oxidation on the surface of $Cr(OH)_3$(s) otherwise under the same conditions produced mixed phase of Mn oxides, consisting of dominantly feitknechtite (β-MnOOH) with minor of groutite (α-MnOOH) and hausmannite. During the redox reactions between birnessite and aqueous Mn(II) under both oxic and anoxic conditions, groutite, feitknechtite, and manganite (α-, β-, and γ-MnOOH, respectively) were produced at pH 7.0, while hausmannite was produced at pH 8.0 and 9.0. Feitknechtite was recognized as the secondary Mn oxide phase during the redox reactions between birnessite and $Cr(OH)_3$(s) at pH 7.0 – 9.0 open to the atmosphere. Overall, the results of this study suggested the potential

geochemical factors controlling the formation and the phase transformation of diverse Mn oxides at different conditions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.O-3**
발표분야: Current Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:30, 좌장: 한승희

Citric acid-Assisted Sequential Redox Process of Tetrabromobisphenol A using Bimetallic Bi/Fe0 Nanoparticles

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POSTECH 환경공학부

Tetrabromobisphenol A (TBBPA) is the most abundantly applied brominated flame retardant. The widespread use of TBBPA and its incomplete removal have led to the release of large quantities of TBBPA into the environment.

This study presents a sequential redox process that uses bismuth-modified nanoscale zero-valent iron (Bi/Fe0) to completely degrade TBBPA. Citric acid (CA) was utilized to enhance the oxidation capability for degradation of TBBPA intermediates over Bi/Fe0 in the presence of oxygen, thereby completely degrading TBBPA.

In the first reduction process, TBBPA and partially debrominated intermediates, including tri-, di-, and mono-bromobisphenol A, were reductively degraded by Bi/Fe0. In the subsequent oxidation process, mono-bromobisphenol A and bisphenol A (BPA) were further oxidized by reactive oxygen species (ROS). CA could promote the bismuth-iron system to produce abundant ROS under oxic conditions due to its ligand function, which could react with Fe(III) to form a ligand complex (Fe(III)Citrate), with considerable production of Fe(II) and H2O2.

This study provides a new strategy for mineralization of many recalcitrant pollutants.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.O-4**
발표분야: Current Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 09:45, 좌장: 황윤정

Charge transfer behaviour of vertically-aligned WO3 microdisc arrays for water oxidation

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One- to three-dimensional alignments of semiconductors on the micro- or nanoscale have been achieved to tailor their opto-physicochemical properties and improve their photoelectrochemical (PEC) performance. Here, we report for the first time the fabrication of vertically aligned, well-ordered WO3 microdisc arrays via an electrodeposition process on lithographically patterned indium tin oxide (ITO) substrates as well as their geometry-specific photoelectrochemical properties. The as-fabricated WO3 microdisc arrays exhibit enhanced light absorption as well as facilitated charge separation, leading to significantly higher PEC performance than that of WO3 films. A finite-difference time-domain simulation of a single WO3 microdisc indicates that the strong optical resonances occur particularly in the central part of the microdisc, leading to enhanced optical absorption. Time-resolved photoluminescence study further reveals that the averaged lifetime of charge carriers in a microdisc array is shorter than that in a film by ~60%. The reductively deposited Au particles are localized on the side of the microdisc and ITO substrate, which suggests that the photogenerated electrons are transferred to the same locations. In addition, the selective oxidative deposition of FeOOH particles on the top surface and side of a microdisc indicates hole transfer pathways at the same locations. This downward transfer of electrons and upward transfer of holes lead to efficient charge separation, and the radial direction appears to be the most preferred shortcut for the carriers inside the bulk of a microdisc.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.O-5**
발표분야: Current Trends in Environmental and Energy Chemistry
발표종류: 구두발표, 발표일시: 목 10:00, 좌장: 황윤정

Highly Selective and Efficient Photoelectrochemical CO2 reduction by Nanoporous Au on Si Photoelectrode

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Photoelectrochemical (PEC) CO2 reduction reaction (CO2RR) has been intensively focused as a promising technology for producing fuel. Up to date, however, poor CO2RR catalysts performance is an obstacle to obtain efficienct PEC cell. We present a Si photoelectrode decorated with a nanoporous Au thin film to achieve highly efficient and selective PEC CO2RR. It includes two important issues as follows. (1) Fabrication of nanoporous Au thin film for co-catalysts We successfully developed nanoporous Au on thin film structure by sequent electrochemical process (anodization & reduction reaction). This developed electrochemical treatment forms induces 20 nm thick nanoporous Au layers on plarnar Au surface. The nanoporous Au layer is observed to compose of a lot of nanoparticles with grain boundaries. For CO2RR performance, dramatically improved CO2 reduction catalytic activity is obtained for CO generation (remarkable selectivity and lowered overpotential) as compared to bare Au thin film. It is very significant that our 20 nm thick nanoporous Au layer shows very exceptional CO2RR activity. (2) Novel design of Si photoelectrode with nanoporous Au thin film To combine the successfully developed nanoporous Au thin film on Si photoelectrode, a novel Si photoelectrode design was proposed by adopting a mesh-type pattering of nanoporous Au thin film. Mesh-type patterned Au thin film is independently wired for electrochemical treatment and the back of the photoelectrode is utilized for Ohmic contact. As the result, our Si photoelectrode decorated by the nanoporous Au thin film exhibits 91% Faradiac efficiency of CO production at -0.03V (vs RHE). We note that this potential is more positive than even CO redox potential (-0.11V (vs RHE). These results should be originated from the superior CO2RR property of the nanoporous Au thin film and generated high photovoltage inside Si substrate. To the best knowledge, it is first time to report high CO2 reduction selectivity (over 90%) at more positive

potential than equilibrium potential. Furthemore, our work provides a general platform of an efficient PEC CO2 conversion cell with adopting various efficient co-catalysts regardless of substrate.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ENVR.O-6**

발표분야: Current Trends in Environmental and Energy Chemistry

발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 황윤정

Poisoning Effects on Ni Electrocatalyst in Solid Oxide Carbon Fuel Cells

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GIST 지구환경공학부

Fuel cells have garnered increasing interest due to concerns about the environmental impact of conventional power generation systems. In particular, fuel cells take advantage of a predictable and continuous power output as long as fuel is sustained or supplied. Meanwhile, it has been occasionally occurred for SO-CFCs (solid oxide carbon fuel cells) that their electrochemical performances go unpredictable and peculiar, leading to not a few limitations on empirical fuel cell operations. In other words, SO-CFC operators can overcome the limitations and improve their system by dint of understating where and why this unwanted results originate from. We have pondered over the origin of the unwanted results and have figured out that it comes from a change in the state of Ni electrocatalyst. Nickel is the most famous electrocatalyst employed in SO-CFCs; however, it could be poisoned by either its oxidation or carbon deposition over its surface. In addition, if Ni is poisoned, an electrochemical performance of SO-CFCs accordingly deteriorates. This poisoning effects stem from the amount of an actual fuel within an anode chamber, i.e. further oxidizable gaseous molecules, the amount of which is determined by the physicochemical properties of solid carbon source. In this regard, we demonstrate a relationship between the physicochemical properties of solid carbon source and the resultant state of Ni electrocatalyst.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-1**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 10:15, 좌장: 권형준

Multi-Functional Transparent Luminescent Configuration for Advanced Photovoltaics

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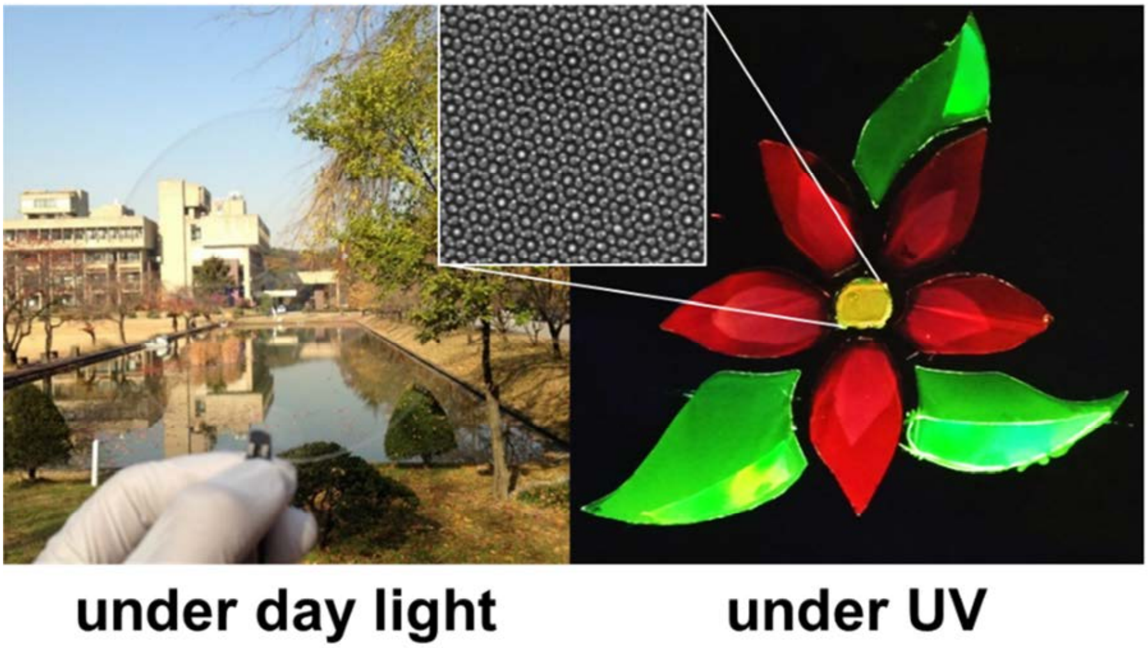
The conversion and manipulation of light via luminescent down-shifting (LDS) show promise in numerous applications. An elegant combination of lanthanide-doped polymer-derived ceramics incorporated with versatile nanopatterns is demonstrated using direct nanoimprint techniques. The prompt formation of nanoscale photonic structures enhances the fluorescence emission from the LDS while retaining the material's optical transparency. The functionality of this material is further expanded to accommodate surface energy modulation by nanopatterns. The practical applicability of this platform in photovoltaic devices is evaluated, showing distinctively enhanced efficiency and lifetime mainly attributed to the nanopattern assisted strong LDS property. Moreover, to efficiently combine two lanthanide emissions, so called a "double imprint" approach is devised by superpositioning two LDS nanopatterned arrays (Figure 1). Combined with the multi-functionality such as prominent LDS characteristics, color tunability, and surface energy modulation, the developed LDS platform offers promise for esthetic building-integrated photovoltaics.

Figure 1. Demonstration of an LDS window. The LDS window was visibly transparent under the ambient condition, whereas a beautiful flower emerged under UV excitation. The red flower was formed using Eu, highlighted by the nanocylinders in the middle areas. The green leaves were formed using Tb also with

appropriate nanocylinders. The center of the sample displayed the double print technique, which mixed and enhanced the red and green fluorescence to achieve a yellow core.



일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-2**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 10:23, 좌장: 권형준

Highly Sensitive, Transparent, and Durable Pressure Sensors Based on Sea-Urchin Shaped Metal Nanoparticles

이동화 이형진 정영준 안유미 남건익 이윤구*

DGIST 에너지시스템공학전공

Pressure sensors have been used for control and monitoring in various electronic applications including force-touching sensors on the display, smart sensors embedded into fabric, medical sensors for health monitoring, and electronic skin. The capacitive and piezoelectric pressure sensors have shown excellent touching sensitivity by employing microstructures. However, they still have several drawbacks such as complex device architecture, low optical transparency, high processing temperature, and restricted scalability because the fabrication of sophisticated microstructures largely depends on complicated and expensive lithographic patterning process. Recently, piezoresistive pressure sensors composed of conductive fillers and insulating elastomers have attracted considerable interest as potential alternatives to the capacitive and piezoelectric pressure sensors. However, most of the piezoresistive pressure sensors still have issues regarding low optical transparency and poor operational durability, which make them difficult for practical use. They are usually opaque because high concentration of non-transparent conductive fillers is required to obtain sufficient piezoresistive characteristics. Therefore, the challenge still remains to develop a novel conductive filler for practical piezoresistive pressure sensors with excellent touching sensitivity, optical transparency, and operational durability. In this talk, I will present a new piezoresistive pressure sensor based on sea-urchin shaped metal nanoparticles and insulating polyurethane elastomer. It showed excellent sensitivity (2.46 kPa^{-1}), optical transparency (84.8% at 550 nm), and operational durability.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-3**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 10:31, 좌장: 권형준

Highly Efficient Green Zn-Ag-In-S/Zn-In-S/ZnS QDs by a Strong Exothermic Reaction for Down-Converted Green and Tripackage White LEDs

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국민대학교 화학과 [1]국민대학교 생명나노화학과

Highly efficient green-emitting Zn-Ag-In-S (ZAIS)/Zn-In-S (ZIS)/ZnS alloy-core/inner-shell/outer-shell quantum dots (QDs) were synthesized using a multi-step hot injection method with a highly concentrated zinc acetate dihydrate (HZAD) precursor. We realized ZAIS/ZIS/ZnS QD growth via five sequential steps: a core growth process, a two-step alloying-shelling process, and a two-step outer-shelling process with regard to band gap engineering along with an enhancement of the photoluminescence quantum yield (PLQY). To enhance the PLQY of ZAIS/ZnS QDs, we added a ZIS inner-shell with a band gap located between the ZAIS alloy core and the ZnS shell using a strong exothermic reaction. The synthesized ZAIS/ZIS/ZnS QDs displayed a high PLQY of 87 % and a peak wavelength of 501 nm. The dual-color down-converted light-emitting diodes (DC-LEDs) that combined the best PLQY ZAIS/ZIS/ZnS QDs and the blue-emitting InGaN LED exhibited a high luminous efficacy (LE) of 154 lm/W at 60 mA. We also realized a tri-package white DC-LEDs using a blue (B) InGaN LED, a green (G) ZAIS/ZIS/ZnS QD-based DC-LED, and a red (R) ZCIS/ZnS QD-based DC-LED. A careful evaluation of the vision and color performance using LE, the color rendering index (CRI), the CRI for strong red (R9), and the external quantum efficiency (EQE) was conducted with the correlated color temperature (CCT) over the range of 2,700 K to 10,000 K. The RGB tri-package white DC-LEDs exhibited high LE (72 lm/W) and excellent color qualities (CRI = 95, R9 = 93, EQE = 0.28) at a CCT of 2,700 K.

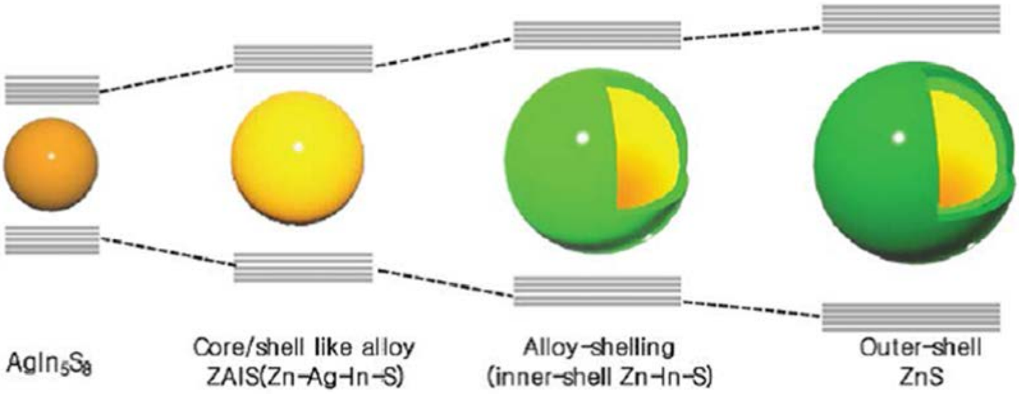

Figure 1. Schematic diagram of band position that consists of core AIS, alloyed core ZAIS, alloy-shelling (inner-shell Zn-In-S), and outer-shell ZnS.

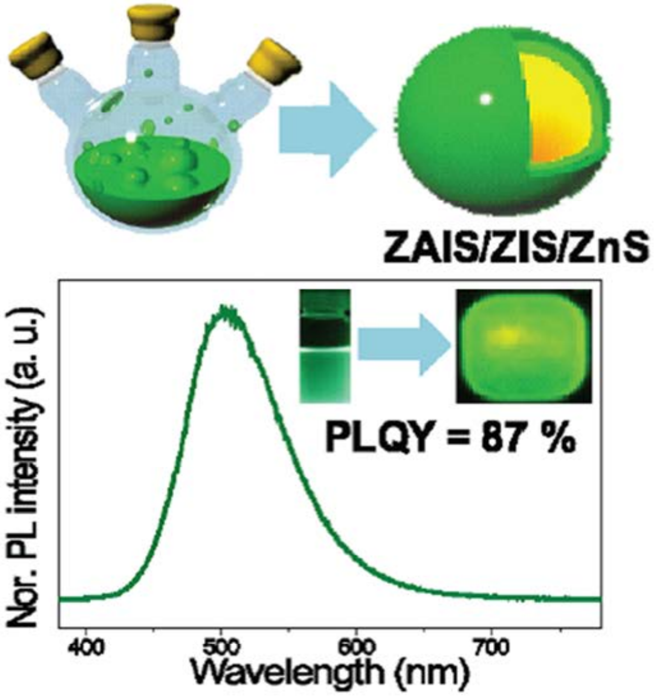

Figure 2. Optical properties of ZAIS/ZIS/ZnS QDs and photograph of emitting ZAIS/ZIS/ZnS QDs solutions and application on InGaN light-emitting diodes using ZAIS/ZIS/ZnS QDs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-4**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 10:39, 좌장: 권형준

A General Approach to Preferential Formation of Active Fe–N_x Sites in Fe–N/C Electrocatalysts for Efficient Oxygen Reduction Reaction

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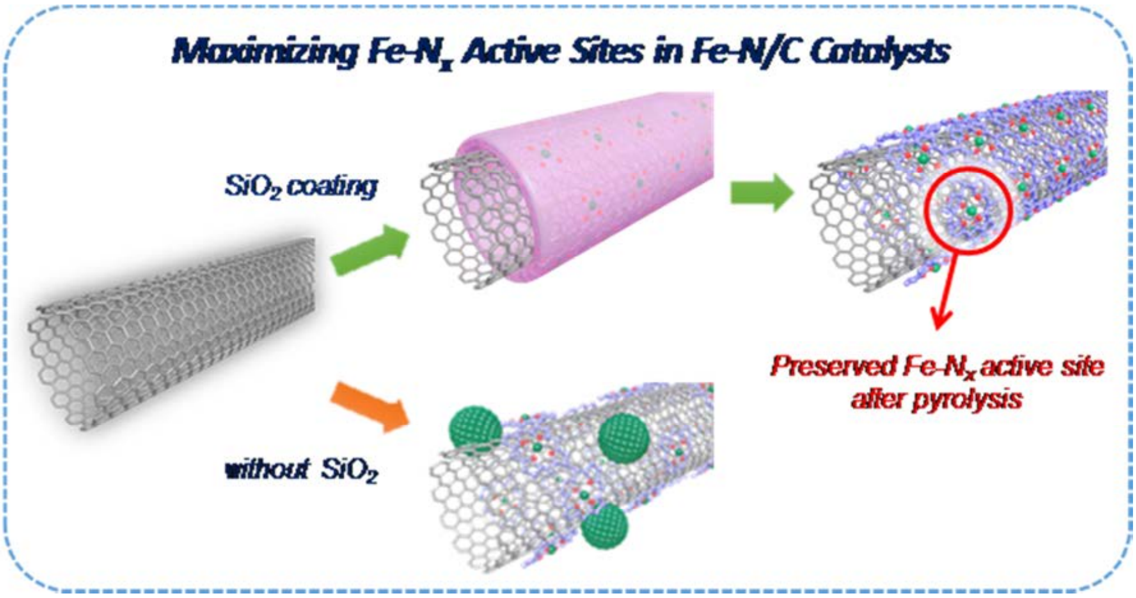
UNIST 화학과 [1]UNIST 에너지화학공학부

Iron- and nitrogen-doped carbon (Fe−N/C) catalysts have emerged as promising nonprecious metal catalysts (NPMCs) for oxygen reduction reaction (ORR) in energy conversion and storage devices. It has been widely suggested that an active site structure for Fe−N/C catalysts contains Fe−N_x coordination. However, the preparation of high-performance Fe−N/C catalysts mostly involves a high-temperature pyrolysis step, which generates not only catalytically active Fe−N_x sites, but also less active large iron-based particles. In this presentation, we present a general “silica-protective-layer-assisted” approach that can preferentially generate the catalytically active Fe−N_x sites in Fe−N/C catalysts while suppressing the formation of less-active large Fe-based particles. The catalyst preparation consisted of an adsorption of iron porphyrin precursor on carbon nanotube (CNT), silica layer overcoating, high-temperature pyrolysis, and silica layer etching, which yielded CNTs coated with thin layer of porphyrinic carbon (CNT/PC) catalysts. Temperature-controlled in situ X-ray absorption spectroscopy during the preparation of CNT/PC catalyst revealed that the coordination of silica layer can stabilize the Fe−N_4 sites. The CNT/PC catalyst contained higher density of active Fe−N_x sites compared to the CNT/PC prepared without silica coating. The CNT/PC showed high ORR activity and excellent stability in alkaline media. Importantly, an alkaline anion exchange membrane fuel cell (AEMFC) with a CNT/PC-based cathode exhibited record high performances among NPMC-based AEMFCs. In addition, a CNT/PC-based cathode exhibited a high volumetric current density of 320 A cm^{-3} in acidic proton exchange membrane fuel cell.


Maximizing Fe-N$_x$ Active Sites in Fe-N/C Catalysts
SiO$_2$ coating
without SiO$_2$
Preserved Fe-N$_x$ active site after pyrolysis

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-5**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 10:47, 좌장: 권형준

Quinoidal Molecules as a New Class of Ambipolar Semiconductor Originating from Amphoteric Redox Behavior

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GIST 신소재공학과 [1]동국대학교 융합에너지신소재공학과 [2]한국원자력연구원 [3]GIST 신소재공학과,나노바이오재료전자공학과

Recently, intensive research of organic electronics based on organic semiconductors has achieved high performance exceeding that of inorganic amorphous silicon. This remarkable progress is attributed to the design and the synthesis of various conjugated molecular building blocks. Conjugated molecules which exhibit high planarity and close stacking are favorable for increasing charge transport property. Among numerous planar molecular building blocks, conjugated molecules based on quinoid structure were focused on in this research. Quinoid structure refers to the aromatic structure linked with double bonds between aromatic rings. In order to retain quinoidal form, specific end group is required. Here, isatin molecule was used as end group for obtaining quinoidal bichalogenophenes. Quinoidal bithiophene (QBT) and quinoidal biselenophene (QBS) were synthesized by short 2 steps. Two small molecules, QBT and QBS, showed low band gap of approximately 1.5 eV in spite of short quinoidal core. Measurement of cyclic voltammetry of QBT and QBS displayed both oxidation and reduction potential; and corresponding highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) level were calculated as 3.7 and 5.3 eV. The organic field-effect transistors based on both quinoidal small molecules showed typical ambipolar behavior arisen from low band gap and amphoteric redox property of quinoidal molecules.

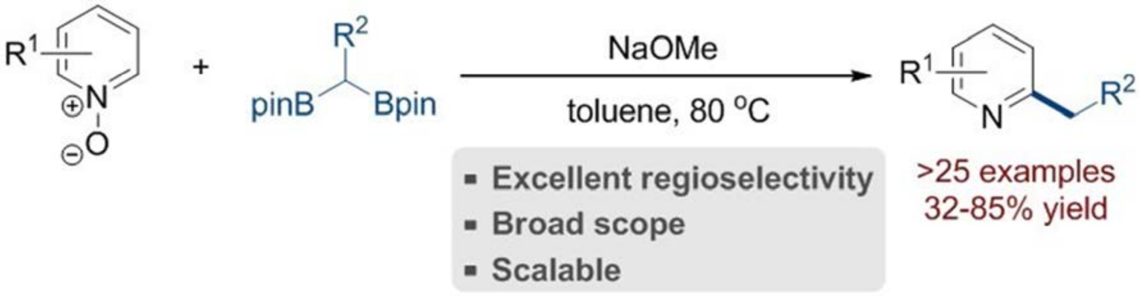
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-6**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 11:00, 좌장: 권형준

Transition-Metal-Free Regioselective Alkylation of Pyridine N-Oxides Using 1,1-Diborylalkanes as Alkylating Reagents

조우현 김정훈 최서영 조승환*

POSTECH 화학과

Reported herein is 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: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-7**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 11:08, 좌장: 권형준

Unprecedented β-Regioselectivity in Cyclopolymerization of 1,6-Heptadiynes Using Grubbs Z-Selective Catalyst

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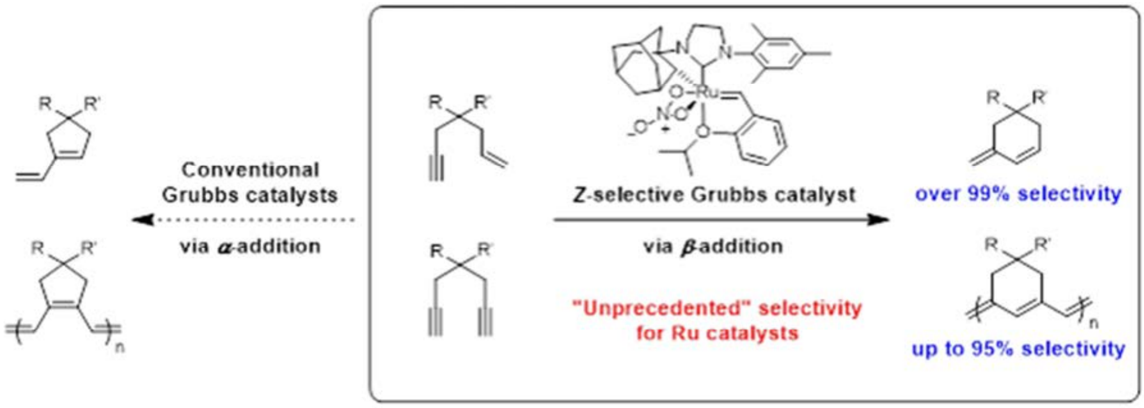
서울대학교 화학부

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 readily accessible and easy-to-use 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 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.


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

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS.O-8**

발표분야: 한국다우케미칼 우수논문상 수상자 구두발표

발표종류: 구두발표, 발표일시: 목 11:16, 좌장: 권형준

Singly and Doubly Occupied Higher Quantum States in Nanocrystals

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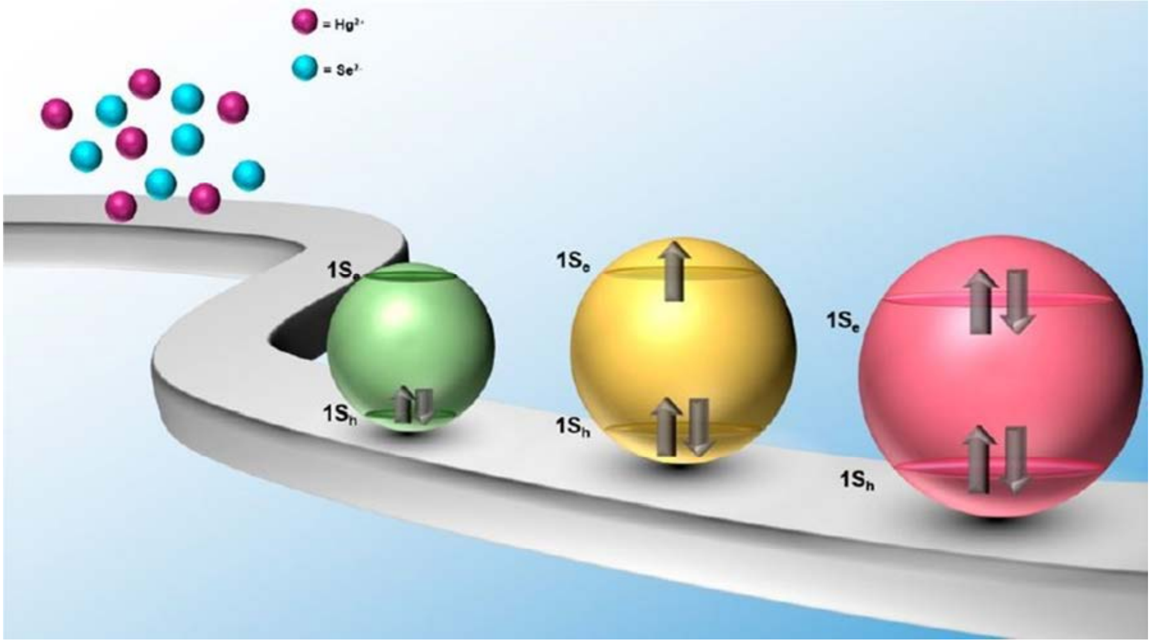
고려대학교 화학과 [1]KU KIST 융합대학원

Colloidal quantum dot (CQD) has been rigorously studied for the last three decades due to its tunable optical and electrical properties by varying the nanocrystal size. Since the CQD is semiconducting material, doping density can determine the CQD device performance. Therefore, it is very important to finely control the doping density of the CQD for manipulating the electric, optical and magnetic properties of CQDs. Previous work has shown the tunable intraband transition of mercury chalcogenide CQD by varying the nanocrystal size. Here, we firstly report HgSe CQDs with zero, one (unpaired) or two (paired) electrons occupying the lowest quantum state of the conduction band (1Se), which has been a long-standing challenge in the colloidal nanocrystal research. The number of electrons in the 1Se state is determined by nanocrystal growth time directly involved in the stoichiometry of the metal-chalcogenide CQD. The singly-occupied-quantum-state (SOQS), when an electron fills the 1Se state in stable under ambient conditions, was confirmed by carrying out the electron paramagnetic resonance spectroscopy. Furthermore, the diamagnetism was observed when zero or two electrons are occupied in the 1Se state, corresponding to doubly-occupied-quantum-state (DOQS). Strikingly, superparamagnetism was identified by performing SQUID for the SOQS HgSe CQDs with varying temperature down to 4 K. The number of electrons in the 1Se state, moreover, can be controlled by surface treatment. The SOQS and DOQS of CQD will be a promising magnetic feature for future spin based applications such as nonvolatile memory, infrared optoelectronics, catalysts, optomagneto-imaging and quantum computing.


= Hg^{2+}
= Se^{2-}
$1S_e$
$1S_h$
$1S_e$
$1S_h$
$1S_e$
$1S_h$

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-9**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 11:24, 좌장: 권형준

Visualization and Quantification of miRNA in a Single cell Using Atomic Force Spectroscopy

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POSTECH 화학과 [1]POSTECH 융합생명공학부 [2]POSTECH 생명과학과

MicroRNAs (miRNAs) play critical roles in controlling various cellular processes, and the expression levels of individual miRNAs can be considerably altered in pathological conditions such as cancer. Accurate quantification of miRNA at the single-cell level will lead to a better understanding of miRNA function. Here, we present a direct and sensitive method for miRNA detection using atomic force microscopy (AFM). A hybrid binding domain (HBD)-tethered tip enabled mature miRNAs, but not premature miRNAs, to be located individually on an adhesion force map. By scanning several sections of a micrometer-sized DNA spot, we were able to quantify the copy number of miR-134 in a single neuron and demonstrate that the expression was increased upon cell activation. Moreover, we visualized individual miR-134s on fixed neurons after membrane removal and observed 2–4 miR-134s in the area of $1.0 \times 1.0\ \mu m^2$ of soma. The number increased to 8–14 in stimulated neurons, and this change matches the ensemble-averaged increase in copy number. These findings indicate that miRNAs can be reliably quantified at the single cell level with AFM and that their distribution can be mapped at nanometric lateral resolution without modification or amplification. Furthermore, the analysis of miRNAs, mRNAs, and proteins in the same sample or region by scanning sequentially with different AFM tips would let us accurately understand the post-transcriptional regulation of biological processes.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-10**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 11:32, 좌장: 권형준

Folding-Generated Molecular Tubes Containing One-Dimensional Water Chains

전해근 정진영 강필재 최문근 정규성*

연세대학교 화학과

We have prepared a series of indolocarbazole-pyridine (IP) foldamers which folded into a helical conformation with an internal tubular cavity. Two repeating units, indolocarbazoles and pyridines, prefer to adopt a *syn*-conformation due to dipolar interactions, and this alternate arrangement of the *syn*-conformations eventually leading helical folding. The upfield shift of aromaric proton signals in 1H NMR spectra shows the pi-pi stacking of aromatic planes due to helical folding. The hyphochromic effect and fluorescence quenching also support the helical folding in solution phase. In solid phase, the X-ray structures clearly showed the helically folded conformations with an internal cylindrical cavity wherein three or five water molecules forming 1D water chains.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **KCS.O-11**
발표분야: 한국다우케미칼 우수논문상 수상자 구두발표
발표종류: 구두발표, 발표일시: 목 11:40, 좌장: 권형준

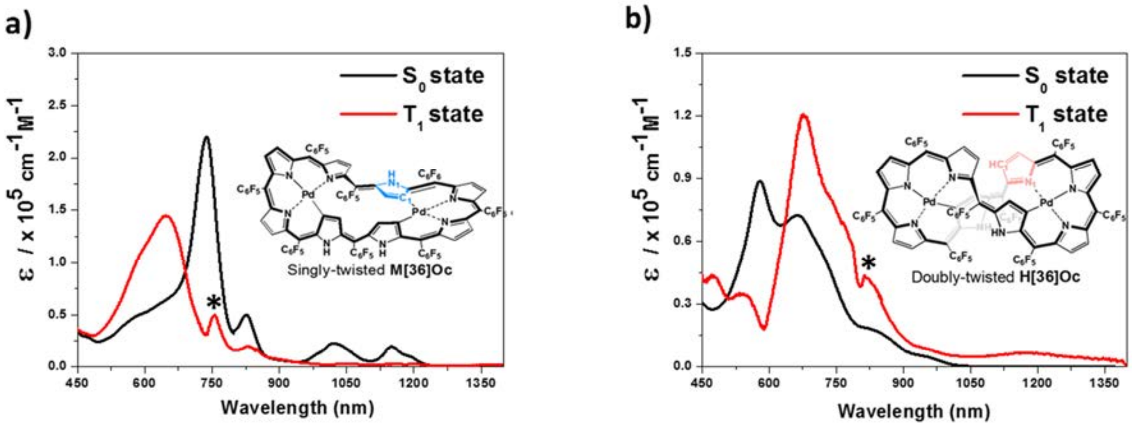
The Extension of Baird's Rule to Twisted Heteroannulenes: Aromaticity Reversal of Singly and Doubly Twisted Molecular Systems in the Lowest Triplet State

홍용석 오주원 성영모 김동호*

연세대학교 화학과

I have investigated the lowest triplet state (T_1) aromaticity of singly-twisted Möbius aromatic and doubly-twisted Hückel antiaromatic bis(palladium(ll)) [36]octaphyrins using spectroscopic measurements and quantum calculations. In the T_1 state absorption spectrum, singly-twisted Möbius [36]octaphyrin showed broad and weak absorption spectral features, which is analogous to those of antiaromatic expanded porphyrins (Fig. 1a). On the other hand, the T_1 state absorption spectrum of doubly-twisted Hückel [36]octaphyrin exhibited intense and distinct features, representing aromatic nature (Fig. 1b). The quantum calculations based on magnetic and topological indices support the reversed aromaticity in the T_1 state. Furthermore, I have revealed that the degree of structural smoothness affects the aromaticity reversal in the T_1 state.

Figure 1. The S_0 and T_1 absorption spectra of a) **M[36]Oc** and b) **H[36]Oc** in toluene. The asterisks indicate experimental errors that are induced by different spectral resolutions between spectrometers used for ground-state absorption and TA measurement.


a)
S0 state
T1 state
ε / x 10^5 cm^-1 M^-1
Wavelength (nm)
*
Singly-twisted M[36]Oc
b)
S0 state
T1 state
ε / x 10^5 cm^-1 M^-1
Wavelength (nm)
*
Doubly-twisted H[36]Oc

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **KCS.O-12**

발표분야: 한국다우케미칼 우수논문상 수상자 구두발표

발표종류: 구두발표, 발표일시: 목 11:48, 좌장: 권형준

[발표취소] Multiscale Hyperporous Silicon Flake Anodes for High Initial Coulombic Efficiency and Cycle Stability

류재건 홍동기 신명수 박수진[1,*]

UNIST 에너지공학과 [1]UNIST 에너지 및 화학공학부

발 표 취 소

본 논문은 발표취소된 논문입니다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-1**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Solid phase extraction of nerve agents' degradation product using polymeric anion exchange film on gold plate

김현석 이봉수[1] 이용한[2,*] 최인성[1,*]

국방과학연구소 제5기술연구본부 [1]KAIST 화학과 [2]국방과학연구소 5본부 3부

The detection of chemical Warfare Agents (CWA) and the related chemicals is important for CWC compliance monitoring. Nerve agent, a kind of CWAs, is hydrolyzed to alkyl phosphonic acid in water and soil. Conventional identification methods such as GC-MS, LC-MS and NMR for alkylphosphonic acids require several steps of sample preparation. In this study, anion exchange film was prepared by surface-initiated polymerization on gold plates using trimethyl ammonium functionalized methacralate to selectively extract alkylphosphonic acids from aqueous samples and analyzed by FT-IR spectroscopy. The prepared plates were immersed in an aqueous samples for 10 minutes and then washed with deionized water for extraction of alkylphosphonic acids. The washed plates were briefly dried in a stream of nitrogen gas prior to FT-IR analysis. FT-IR was able to successfully analyze concentration samples at ppm levels.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-2**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Control of the Hydrophobic and Electrostatic Interaction between Molecular Beacon Aptamer and Conjugated Polyelectrolyte for Detection Range-Tunable ATP Assay

정지은 우한영*

고려대학교 이과대학 화학과

Electrostatic and hydropobic interactions between cationic conjugated polyelectrolytes (CPEs) and molecular beacon aptamer (MBA) makes MBA to have conformation of either open chain or G-quadruplex depending on the presence of a target. MBA is labelled with a fluorophore and a quencher at both termini. In the absence of a target, MBAs have open chain conformation with CPEs, enabling facile FRET from the CPEs to a fluorophore in MBA. By forming a G-quadruplex with a target, strong interaction between the MBA and target ensures the close contact between fluorophore and quencher, resulting in quenched PL signal. Here we report a new strategy of detection range modulation in the CPE-MBA based assay with different stem strength. Modification of ionic density of CPEs suggests an efficient way to fine-control the assay characteristics like detection range and limit of detection.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-3**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Efficient thermoelectric system using conducting polymers by doping

조성준[*] 우한영[1,*]

고려대학교 화학 [1]고려대학교 이과대학 화학과

*Sungjoon Cho[1] , Jiae [1], Thanh Luan Nguyen[1], HanYoung Woo[*1] Department of Chemistry, College of Science, Korea University, Seoul 136-713, Republic of Korea[1] hywoo@korea.ac.kr*[*]Since organic polymers-based thermoelectric devices have advantages of light weight, mechanical flexibility, room temperature solution fabrication, and lower thermal conductivity compared to inorganic devices, researches on thermoelectric devices based on polymers is very promising. We synthesized new conjugated polymer based on cyclopentadithiophene (CDT) by suzuki coupling. Furthermore we studied its UV-vis spectra, electrical conductivity and resulting thermoelectric characteristics by chemical doping with tris(pentafluorophenyl)borane. In the UV-vis spectra, we observed the increasing tendency for the peak around 1000nm with increasing concentration of dopant. The electrical conductivity was also increased about 6 times than pristine, and the optimized power factor up to 6.15 μW/mK2 was measured.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-4**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Cotable Polarizer Fabricated by Polymer-Stabilized Chromonic Liquid Crystals

최유진 정광운[1,*]

전북대학교 고분자 나노공학과 [1]전북대학교 고분자.나노 공학과

A chromonic liquid crystal (CLC) polarizer was fabricated from Sunset Yellow FCF (H-SY) Macroscopic molecular orientation was achieved by bar-coating the self-assembled lyotropic CLCs and the oriented structure was frozen by the subsequent photo-polymerizing processes. Their molecular packing structures and optical behaviors were further investigated using the combined techniques of microscopy, scattering and spectroscopy. The polymer-stabilized H-SY films showed good mechanical and chemical stabilities without sacrificing a high polarizability. Therefore, it can allow us to develop the smart optical and electrical devices. This work was supported by the MOTIE/KDRC 10051334, BK21 Plus program, Mid-Career Researcher Program (2016R1A2B2011041), and Global Ph. D. Fellowship Program (NRF-2016H1A2A1907561) of Korea.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-5**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Striped Patterned Polymer Network from Discotic Reactive Mesogen

정다슬 정광운[1,*]

전북대학교 고분자.나노공학과 [1]전북대학교 고분자.나노 공학과

A triphenylene-based reactive mesogen molecule (abbreviated as TPBRM) was newly designed and synthesized for the fabrication of striped walls during photopolymerization in the anisotropic liquid crystal (LC) medium. From thermal, scattering and microscopic results, it was found that TPBRM formed three ordered structures: a columnar hexagonal LC phase, a tilted columnar hexagonal LC phase and a highly ordered columnar oblique crystal phase. While the dimensions of the striped wall morphologies were determined by the patterned photomasks, the microscopic molecular orientations in the hierarchical superstructures were self-organized with the support of surface anchoring forces. Regardless of the photomask direction, the long axis of self-assembled columns in the striped walls was normal to the surface alignment direction. In addition, it was realized that the shapes of water drops as well as the surface contact angles of the surface water can be controlled by the hierarchical superstructures and morphologies of the polymerized TPBRM networks. The fabricated hierarchical superstructures and morphologies can allow us to develop electronic and microfluidic devices. This work was supported by the BRL 2015042417, LHRT 2016H1D5A910159 Regional Neo Industry Program, Mid-Career Researcher Program 2016R1A2B2011041 and the BK21 Plus program.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-6**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Facile Fabrication of Flexible Photonic Crystals by Controlled Helicoidal Superstructure of Self-Assembled Chiral Polymers

김대윤 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

Photonic crystals unveiled in nature offer chemists to inexhaustible opportunities to develop the novel materials to tune the reflective colors. Synthetic opal and colloidal crystal have been extensively studied. Recently, material scientists have tried to develop the flexible optical films and fibers for applying in the advanced displays with portability and wearability.Along this line, polymers self-assembled into the helical superstructures have been widely discussed because they possess not only the orientational properties of anisotropic molecules but also the elastic properties of polymeric networks. Here, we report the example of free-standing red, green, and blue color reflection film. The helical superstructures are effectively networked by the in situ polymerization of chiral monomers. This work was mainly supported by MOTIE and Mid-Career Researcher Program of Korea.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-7**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

From Smart Denpols to Logic Devices

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Dendronized polymer (denpol) is newly designed and successfully synthesized by ring-opening metathesis polymerization (ROMP) of norbornene-based dendrons containing azobenzene-functionalized components and their self-assembly to produce the photomechanical work is systematically investigated. The uniaxially oriented film forms the well-ordered lamellar superstructure. The free-standing film is found to show the photorevesible actuating motion upon alternating the wavelength of irradiation light. The observation of peculiar bending direction from this material highlights that photomobile behavior can be precisely controlled in the defined manner by manipulating the hierarchical symmetry of the initial chromophore alignment. The photorevesible bending and unbending motion with a praogrammed direction will be beneficial for the practical application of the remote-controllable wireless actuator and light-switchable logic devices. This work was mainly supported by MOTIE and Mid-Career Researcher Program of Korea.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-8**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Multi-stimuli Responsive Photochromic Molecules with Chiral Naphthyl-based Azobenzene Moieties

황주경 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

For the development of chameleon-like color changeable molecules with respect to various external stimuli, a photochromic chiral molecule with (R)-configuration naphthyl moiety and azobenzene mesogens (abbreviated as CNA_2M) was newly designed and synthesized. From thermal and microscopic analyses, the basic phase transition behaviors of CNA_2M were first studied. It was recognized that CNA_2M formed a tilted version of a highly ordered smectic crystal phase with a layered structure based on structure-sensitive X-ray diffraction results. By doping the CNA_2M chiral molecule into an achiral nematic liquid crystal (LC) medium, chiral nematic (N^*) LC phase with helical superstructures were formed. The reflection colors of N^*-LC films were precisely tuned by changing the helical pitch length of N^*-LC responding to temperature, light and electric field. The multi-stimuli responsive chameleon molecule may allow us to fabricate the reversible modulating devices including remote-controllable photo-responsive devices covering the whole visible region. This work was mainly supported by BRL (2015042417), MOTIE (10047806), Mid-Career Researcher Program (2016R1A2B2011041), and BK21 Plus program, Korea.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-9**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

PDDA/urushi IPN 음이온 교환 전해질 막 제조 방법에 따른 특성 연구

김동영 조혜진 원종옥*

세종대학교 화학과

음이온 교환 전해질 막 (anion exchange membrane, AEM)은 알칼리 연료전지, 물 분해를 통한 수소 제조 및 레독스 흐름 전지 등 다양한 에너지 변환 및 저장장치의 핵심 소재로, 화학적 안정성 및 높은 이온 전도도, 이온 선택도가 요구된다. 따라서 음이온 교환 특성이 있는 polydiallyldimethylammonium chloride (PDDA)를 화학적 안정성이 높은 urushi matrix 에 도입하여 PDDA/urushi 전해질 막을 개발하였다. Urushi 는 천연 옻나무 수액의 주성분인 urushiol 의 가교반응에 의해 얻어지는 crosslinked matrix 로 높은 열적/화학적 안정성을 갖고 있다. Uirushiol 은 상온에서 락카제 효소에 의한 가교 반응 만이 아니라, 열, 광 등에 의해서도 가교가 되는 특성이 있다. 어, 고분자인 PDDA 와 단량체인 Diallyldimethylammonium chloride 을 이용하여 각각 semi-IPN, IPN 구조의 전해질 막을 제조하였다. 열 가교 방법과 수분, 효소에 의한 다양한 가교 방법으로 PDDA/urushi 전해질 막을 제조하고, 반응 조건에 의한 PDDA/urushi 전해질 막의 특성을 분석하였다. Urushi 및 PDDA 합성은 FT-IR 로 확인하였고, 반응 조건에 따른 메커니즘을 분석하였다. 막의 물리적 특성은 Swelling test, Electrolyte Uptake, SEM, TGA 등을 통해 분석하였다. semi-IPN 이나 IPN 의 구조에 상관없이 PDDA/urushi 막에서 PDDA 의 양이 증가할수록 이온 전도도는 향상되고, 이온 선택도도 증가하였다

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-10**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

수계 바나듐 레독스 흐름 전지용 Nafion/urushi 복합막

정지윤 원종옥*

세종대학교 화학과

풍력, 태양에너지 등은 화석연료를 대체할 유망한 에너지 원천이지만, 이를 이용한 신재생에너지는 환경에 따라 영향을 받아, 스마트 그리드 시스템에 적용하기 위해 바나듐 레독스 흐름 전지 (VRFB)와 같은 에너지 저장 장치에 대한 연구가 활발히 진행되고 있다. 수계 VRFB 에서 널리 사용되고 있는 나피온 같은 양성자 교환막은 양극 전해질과 음극 전해질을 분리시켜주며 전지의 성능을 결정하는 중요한 구성요소이다. 수계 VRFB 에서 사용되고 있는 나피온막은 화학적으로 안정하고 이온전도도가 높지만 수계 전해액에서 이온 채널이 팽윤되어 활성종이 투과해 VRFB 의 쿨롱 효율이 낮아지는 주된 원인이다. 따라서 본 실험에서는 화학적으로 안정하고 뛰어난 내구성을 갖는 urushi 를 도입한 나피온을 제조하여 활물질의 투과도를 낮춰 향상된 VRFB 효율을 얻었다. urushi 를 2.1wt% 함유한 나피온/urushi 복합막의 이온 전도도는 0.6 S/cm 이고, 투과도는 7.36×〖10〗^7 〖cm〗^2/min 으로 나피온보다 낮은 값을 보였으며, urushi 함유량이 증가할수록 낮은 투과도를 나타내었다. Swelling test 와 water uptake test 를 통해 나피온/urushi 복합막이 나피온 212 막보다 낮은 팽창률과 흡수율을 보였다. TGA 로 열적 안정성을 확인한 결과, VRFB 작동 온도에서 나피온보다 높은 열적 안정성을 보였다. VRFB 의 충방전 테스트 결과, Urushi 가 3.2wt% 들어간 나피온의 쿨롱효율은 95.0%, 에너지효율은 91.0%으로 나피온 212 를 사용한 VRFB 보다 각각 21.8%, 22.6% 증가하였다. 따라서 urushi blocking 물질이 도입된 나피온/urushi 막의 VRFB 응용 가능성이 매우 높아 차세대 에너지 발전에 많은 기여가 될 것이다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-11**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

HNT 나노 튜브를 이용한 음이온 교환 막의 제조 및 특성 연구

최라영 김동영 원종옥*

세종대학교 화학과

화석 연료의 고갈 및 지구온난화 문제 해결책인 신재생 에너지를 저장하기 대용량 에너지 저장이 가능하고, 높은 안정성과 넓은 전압 범위를 가지는 레독스-흐름 전지 (Redox flow battery, RFB)가 활발히 연구되고 있다. 레독스-흐름 전지는 활성종의 산화, 환원에 의하여 에너지를 저장할 수 있다. 레독스-흐름 전지의 주요 구성요소인 이온 전해질 막을 개발하고, 막의 특성을 연구하였다. 전지 내부의 효율을 결정하는 중요한 소재인 이온 전해질 막은 양극과 음극 전해질을 분리시키면서, 선택적으로 이온을 투과시킬 수 있어야 한다. 또한 각 극에 있는 산화-환원 활성종은 투과시키지 않으면서, 지지 전해질을 통과시켜야 하므로 이온 전도도가 높아야 하고, 화학적/기계적 안정성이 높아야 한다. 따라서 기계적 강도와 열적 안정성이 우수한 Halloysite nanotubes (HNT)에 Urushiol 과의 UV 가교 및 이온 전달 site 를 가진 amino 기를 도입하기 위해 HNT 에 3-aminopropyltriethoxysilane 를 이용하여 rod 형태의 이온 전달기를 제조하고, 이를 내구성이 강한 matrix, 즉 urushi 에 도입하여 이온 교환막을 개발하였다. Urushi 는 천연 옻 소재인 urushiol 을 HNT-NH2 존재하에서 UV 가교 및 열가교 반응을 통해 합성하였고, 개발된 HNT-NH2/urushi 막은 FT-IR, TGA, SEM, WAXS 등으로 물리적 특성을 확인하고, 이온 전도도, 바나듐 투과도 등을 측정하여 레독스-흐름 전지에 응용가능성을 확인하였다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-12**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of multi-arm PEG-based hydrogel

배세원

한국생산기술연구원 청정생산시스템연구소/그린공정소재그룹

Hydrogel is a three-dimensional crosslinked polymer that has found a wide range of applications, from drug delivery to regenerative medicine, because of its similarity to body tissues, its applicability to only the infinitesimal damaged regions, its controlled drug release rate, biodegradability, high water content. In particular, advances in polymer synthesis and processing have led to the next generation of dynamic systems that are capable of responding to biological signals with artificial triggering and spatial accuracy.In this presentation, we will report the synthetic strategy of the monomer and the detailed procedure of multi-arm PEG-based hydrogel synthesis. The effect of cross-linking degree to swelling ratios will also be discussed.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-13**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Highly efficient perovskite solar cells with long-term stability using dopant-free polymeric hole transporting materials

강경호 박태호*

POSTECH 화학공학과

Hole transporting materials (HTMs) must be further developed to achieve high power conversion efficiency and stability in perovskite solar cells. We report a novel D–A polymeric HTM based on benzo[1,2-b:4,5:b']dithiophene (BDT) and 2,1,3-benzothiadiazole (BT), which results in highly efficient and stable perovskite solar cells. The hole mobility of synthesized polymeric HTM,RCP was 3.09 x 10^-3 cm^2 V^-1 s^-1 without any dopants. The RCP-based perovskite solar cell exhibits the highest efficiency (17.3%) in the absence of dopants [lithium bis(trifluoromethanesulfonyl)imide and tert-butylpyridine]. In addition, the long-term stability of the device is dramatically improved by avoiding deliquescent or hygroscopic dopants and by introducing a hydrophobic polymer layer. RCP devices maintain their initial efficiency for over 1400 h at 75% humidity, whereas devices made of HTMs with additives fail after 900 h.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-14**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Marine Antifouling Applications of Dextran-Coated Solid Substrates

정연우 강성민*

충북대학교 화학과

Control over marine biofouling on artificial surfaces has been of interest because undesired fouling of marine organisms onto marine vessels and equipments leads to disturbance of marine ecosystem and increase of fuel consumption. Much effort has been made to find methods for marine antifouling coatings. Dextran, which is one of natural polysaccharides, has been known as effective antifouling materials. For example, mammalian cell- and bacteria-repellent property of dextran-coated substrates were previously reported. However, marine antifouling property of dextran-coated substrates has not been fully investigated, yet. In this study, we demonstrate a method to suppress marine fouling using the dextran coating. Dextran was conjugated with catechol, and the resulting material was used for surface coating of solid substrates. The marine antifouling property of the surface was confirmed using marine diatom adhesion assays, which revealed that the dextran coating reduced diatom adhesion.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-15**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, Characterization, and Photovoltaic Properties of New Two Dimensional Benzodithiophene(BDT)-based Copolymers

김지영 이상규[1] 신원석[1] 강인남[*]

가톨릭대학교 화학과 [1]한국화학연구원 에너지소재연구센터

A new donor-acceptor (D-A) conjugated copolymer based on benzodithiophene (BDT) and thieno[3,4-c]pyrrole-4,6-dione (TPD) was synthesized via a Stille cross-coupling reaction. A highly conjugated thiophene-based side group is incorporated into each BDT unit to generate a two-dimensional (2D) D-A copolymer (P1). As a control, the alkoxy-substituted BDT-based TPD copolymer (P2) was synthesized using the same polymerization method. The polymers were well soluble in common organic solvents, such as chloroform, chlorobenzene, etc. P1 thin films produce two distinct absorption peaks. The shorter wavelength absorption (475 nm) is attributed to the BDT units containing conjugated thiophene-based side groups, and the longer wavelength band (566 nm) is due to the intramolecular charge transfer between the BDT donor and the TPD acceptor. The UV-visible absorption spectrum of P2 in the film state also contains two λmax at and 410 nm, however, the intensity of the shorter wavelength peak is very weak. The highest occupied molecular orbital (HOMO) energy levels of P1 and P2 were calculated to be –5.45 and –5.40 eV, respectively. The LUMO levels of P1 and P2 were calculated to be –3.58 and –3.49 eV, as estimated from the optical band gaps and HOMO energy levels. The organic photovoltaic properties of these polymers will be studied.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-16**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Analysis on Forming 3-D Effective Charge Transport Pathway in Diketopyrrolopyrrole-Based Copolymers via Controlling of Side Chain Bulkiness

김상원 손성윤 박태호*

POSTECH 화학공학과

To achieve high processability and planarity, we have newly designed and synthesized novel series of copolymers based on 2,2′-(2,5-dialkoxy-1,4-phenylene)dithieno[3,2-b]thiophene (TT-P-TT) for donor units with various bulky side chains and diketopyrrolopyrrole (DPP) for acceptor units. These copolymers have a highly planar backbone derived from intramolecular interactions. We have investigated the effects of intermolecular interactions on packing structures, thin-film morphologies, and charge transport by controlling the side chain bulkiness of copolymer. Charge transport dynamics of the copolymer based field-effect transistors (FETs) has been investigated. The thin-film microstructures of the copolymers are dependent upon subtle changes in the intermolecular interactions. The copolymer with the smallest side chain shows remarkably high charge carrier mobility, although the size of the fibrillar structures increases as the bulkiness of the side chains in the copolymer increases. Our findings show the condition for forming effective 3-D charge transport pathway and the importance of the molecular packing and interdomain connectivity, rather than the crystalline domain size. The results demonstrate the importance of the side chain bulkiness and provide new insights into the molecular design for high-performance polymer semiconductors.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-17**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of nanoporous polymer films based on photoinitiated polymerization-induced microphase separation process

오재훈 서명은*

KAIST 나노과학기술대학원

Nanoporous polymers with three-dimensionally continuous pore structure are beneficial in many applications as diffusion through the interconnected porous space is facilitated. Here we report such nanoporous polymers with tunable mechanical properties can be readily fabricated as free-standing films via photoinitiated polymerization-induced microphase separation (photoPIMS) method. In contrast to thermally initiated polymerization that requires high polymerization temperature and lengthy polymerization time, we will show that photoPIMS process allows production of crosslinked block polymer films at ambient temperature with short polymerization time, and subsequent etching of the sacrificial block from the film results in the desired nanoporous film. We will further demonstrate elastic nanoporous films can be fabricated by adjusting the composition of the polymerization mixture for the photoPIMS.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-18**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Thin Film Properties of A 4-(1,2,2-trifluorovinyloxy)benzoyl Substituted Polyimide for Gate Insulator in Thin Film Transistor

기경민 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: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-19**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Thin Film Properties of Novel Crosslinked Polyimide Gate Insulators for Thin Film Transistor with Ultra-Low Leakage Current Density

기경민 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.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

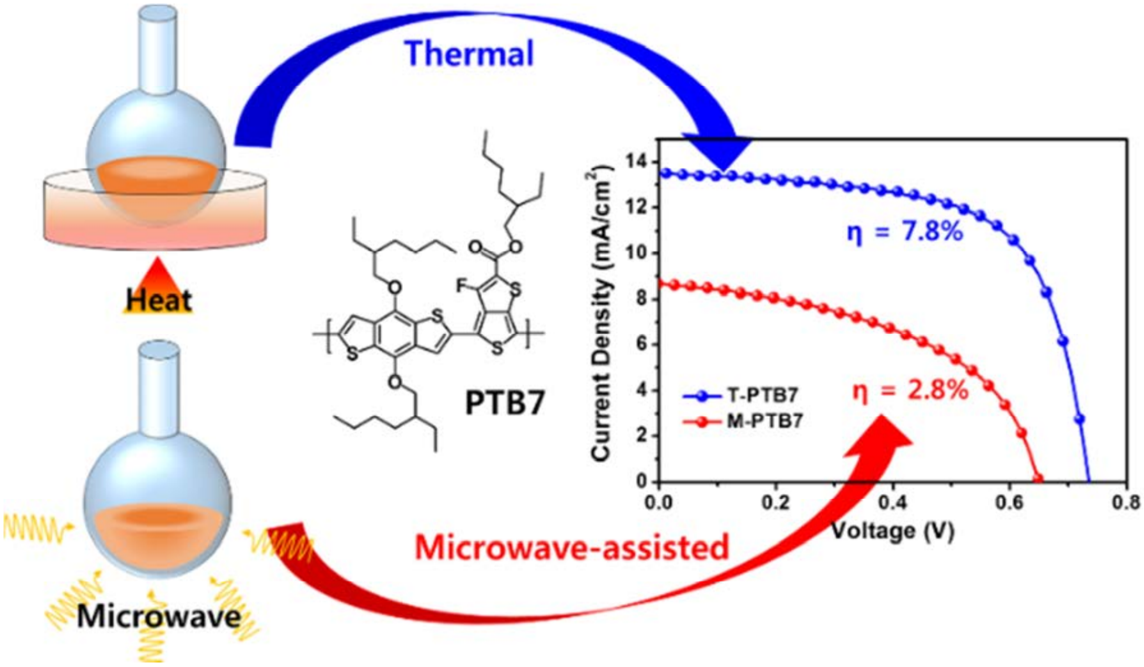
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-20**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The effects of microwave-assisted polymerization on a benzodithiophene(BDT)-based D-A conjugated polymer (PTB7) for the polymer solar cells

박철웅 손성윤 김태완 김상원 박태호*

POSTECH 화학공학과

We report a comparative study on the thermal- and microwave-assisted Stille-coupling polymerization of a benzodithiophene-based donor–acceptor polymer (PTB7). We synthesized three PTB7 polymers through Stille-coupling polymerization under microwave conditions (M-PTB7(32k) and M-PTB7(75k)) as well as thermal conditions (T-PTB7(31k)) for this study. The microwave-assisted polymerization is a powerful methodology to increase the M_n of PTB7 without broadening D in a short time. However, M-PTB7(32k) exhibited a lower PCE of 6.1% compared with that of T-PTB7(31k) (7.8%). Interestingly, the higher molecular weight of M-PTB7(75k) under microwave-assisted conditions resulted in a significant reduction in the device performance (PCE of 2.8%). The microwave-assisted polymerization method accelerated the formation of homo-coupled units that act as charge-trapping sites in PSCs comprising a blend of M-PTB7 and $PC_{70}BM$, which in turn resulted in a decrease in J_{sc} and FF values for M-PTB7.The increased abundance of these homo-coupled units under the microwave-assisted conditions was demonstrated by various optical spectroscopy and the model reaction study.


Thermal
Heat
Microwave
Microwave-assisted
PTB7
F
S
O
Current Density (mA/cm^2)
Voltage (V)
η = 7.8%
η = 2.8%
T-PTB7
M-PTB7
0.0
0.2
0.4
0.6
0.8
0
2
4
6
8
10
12
14

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장소: 일산 KINTEX
발표코드: **POLY.P-21**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Contact type Triboelectric Nanogenerator using PEIE polymer to changing potential state

김태완 박태호*

POSTECH 화학공학과

We suggest new method to change the surface potential of metal surface using PEIE polymer. The shifted work function of electrode makes more driving force of electrons, which lead to more high open circuit voltage and short scircuit current of triboelectric nanogenerator(TENG). This nanogenerator finally report the 50.6% increased output power density without any change of electrical characteristic of contact polymer.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-22**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Photo-switchable Liquid Crystal Alignment by photo-polymerized Amphiphilic isomer

윤원진 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

A synthesized photo-polymerized amphiphilic isomer (abbreviated as ADMA1) was successfully applied as a robust photo-switchable LC alignment layer by self-assembly and photo-isomerization without the conventional polymer-based liquid crystal (LC) alignment process. The LC alignment layer constructed by directly adding photo-polymerized amphiphilic isomer into LC media significantly cuts the manufacturing cost as well as opens new doors for the fabrication of novel electro-optical devices. This work was supported by the BRL 2015042417, MOTIE/KDRC 10051334, Mid-Career Researcher Program (2016R1A2B2011041), and BK21 Plus program of Korea.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-23**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Dual Photo-Functionalized Hierarchical Superstructures for Optically Tunable Thin Film

이유민 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

For the fabrication of optically tunable multifunctional thin films, was newly designed and synthesized a dual photo-functionalized hierarchical superstructure (abbreviated as AZDAA) containing azobenzene and diacetylene groups. Based on the combined experimental results with DSC, POM, SAXS and WAXD, we confirmed the phase behaviors and molecular packing structures. Since the photo-isomerization of the azobenzene moiety, the liquid crystalline phase was transformed from ordered smectic A (SmA) to disordered Isotropic (Iso) phase under the UV light. And due to the photo-polymerization of the diacetylene moiety in solid state, the thermos-reversible color changing was observed by irradiating UV light. We demonstrated the dual photo-functionalization of AZDAA as remote-controllable light shutter, photo-patterned thin film, and thermo-responsive color switch. This work was supported by, the MOTIE/KDRC 10051334, BRL 2015042417 and the BK21 Plus program.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-24**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and characterization of anti-biofouling copolymers consisting of cyclotetrasiloxane derivative

하종운 황도훈*

부산대학교 화학과

Random copolymers consisting of cyclotetrasiloxane (CTS) were designed and synthesized for anti-biofouling. Random copolymers such as poly(styrene) (PS), poly(styrene-r-cyclotetrasiloxane) (PS-CTS), and poly(cyclotetrasilaxne) (PCTS) were synthesized, with different monomer ratios, by radical polymerization. The properties of PS-CTSs and PCTS were compared with polystyrene (PS). The synthesized CTS monomers and copolymers were characterized by proton nuclear magnetic spectroscopy (1H-NMR), gel permeation chromatography (GPC), respectively. Protein adsorption experiments on the polymer surfaces were carried out using fluorescein isothiocyanate conjugate labeled bovine serum albumin. Experimental results suggest that the surfaces of the consisting of cyclotetrasiloxane copolymers have a good anti-biofouling effect.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-25**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Characteristics of Conjugated Small Molecules with Broadband Solubility for Organic Optoelectronic Devices

정재훈 김화정 김영규*

경북대학교 화학공학과

Solution-processable organic optoelectronic devices, such as organic photodetectors and organic solar cells, have attracted keen interest owing to their benefits including low-cost manufacturing and high design freedom. Of various organic semiconducting materials for such organic optoelectronic devices, conjugated small molecules have been recognized to take better advantages than conjugated polymers in terms of molecular purity with an exact (uniform) molecular weight. Our group has recently been involved in synthesizing series of conjugated small molecules and their applications for organic photodetectors and organic solar cells. Some of our approaches have reached diketopyrrolopyrrole derivatives that have beneficial optical absorption in a long wavelength range. This presentation is going to introduce synthesis of particular conjugated small molecules with a wide spectrum of solubility and discuss their applications to organic optoelectronic devices.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-26**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Pt (IV)-Crosslinked PEI Structure for Redox-Triggered Anticancer Drug/siRNA Delivery

정성진 김원종[1,*]

POSTECH 시스템생명공학부 [1]POSTECH 화학과

For overcoming the drawbacks of conventional Platinum (II)-based anticancer drugs, Platinum(IV)-based ones have exhibited enormous potential as cancer therapeutics. In addition, the axial position of Pt(IV) has two reaction sites for the crosslinking of two molecules. We present a Pt(IV)-based polymer structure for synergistic siRNA and cisplatin delivery. To achieve this, low molecular weight polyethylenimines (PEIs) were crosslinked by the axial position of Pt(IV), and poly ethylenglycol (PEG) was subsequently conjugated to formulate the polymer structure (Pt-PEI-PEG). The Pt-PEI-PEG exhibited redox-responsive dissociation of polymers and the simultaneous release of active Pt(II) drug, resulting in not only faster gene release but also high drug efficacy. Efficient delivery of siRNA using Pt-PEI-PEG was monitored in cellular level. By employing siBcl-2 which enhances the apoptosis caused by anticancer drugs, synergistic therapeutic effect of cisplatin and siRNA was demonstrated.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **POLY.P-27**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Graphene-polypyrrole nanocomposites for electromagnetic microwaves absorption

<u>VU THI QUYEN</u> 손대원* Ngo Trinh Tung[1,*]

한양대학교 화학과 [1]Vietnam Academy of Science and Technology, Institute of Chemistry

Conducting nanocomposites of polypyrrole have been attracted interesting because of their various applications in sensors, memory devices and electromagnetic microwave absorbers. In this study, graphene/polypyrrole nanocomposites were synthesized by in situ method with varying polymerization time to observe how reaction time effects on conductivity of resultant nanocomposites. Experimentally, the conductivity of nanocomposites showed increasing as increasing of reaction time. The morphology was investigated by SEM while chemical components were defined by FT-IR and Raman spectroscopy. The thermal stability of nanocomposites was studied using thermogravimetric analysis (TGA) method. For microwave measurement, nanocomposites were mixed with 20% wt epoxy resin and pressed into a 10cmx10cm mold at different thickness from 1.5mm to 3mm. The vector network analyzer in the range from 8GHz to 12GHz was used to define microwave absorbing performance of nanocomposites.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-28**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Injectable Matrix for Neuronal differentiation of Tonsil Derived Mesenchymal Stem Cell

PATELMADHUMITA 고두영 정병문*

이화여자대학교 화학나노과학과

Currently stem cell therapies are investigated as a solution for many neurological diseases. Many clinical trials are processing to either replace lost neuron populations or provide supporting glial cells, but unfortunately no stem cell based therapies have been able to move to the market of clinic due to failure or show no improvement in humans and limited cell characterization. In the current study, poly (ethylene glycol)-poly (L-alaline)-poly (L-aspartate) (PEG-PA-PD) was studied for neuronal differentiation of Tonsil Derived Stem Cell (TMSC). The result suggests that 13µM is best IKVAV concentration for 3D neuronal differentiation out of 26 µM, 66 µM, and 134 µM concentration of peptide. Neuronal differentiation was confirmed by both mRNA and protein expression level of neuronal biomarker like microtubule associated protein-2, tubulin beta-3, glial fibrillary acidic protein and neurofilament-M. This work demonstrates that hydrogel with peptide provide a tunable platform which can improve the culture conditions for neuronal maturation and integration and enhanced stem cell therapies.

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장소: 일산 KINTEX
발표코드: **POLY.P-29**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of flexible, sensitive pressure sensor based on carbon nanotube nanocomposite

조수민 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Devices made from stretchable electronic materials are under huge interest as future application for wearable device in means for clothing or directly attached sensor. Such materials have typically been prepared by engineering elastomeric materials such as silicon.[1] Here we studied flexible and highly sensitive pressure sensor using thin films of carbon nanotube. CNT-PDMS nano composite based pressure sensors were tested on silver nanoparticle electrode array fabricated by printing method. Four composite films with different CNT concentration were fabricated by bar coating and 2mm pads were made from each of them. PDMS spacer is placed on the substrate and rigid PDMS top-plate is covered. By creating gap between electrode and CNT pad sensor using PDMS wall the sensitivity increases and electric read-out differs following the size of the composite and spacer design. Patterned CNT pad works as a sensor when it touches the electrode on the substrate when the top-plate is compressed. The silver nano particle ink was used to draw electrode by Sonoplot. By applying printing method, large area of substrate can be dispensed easily in short time with minimum error regardless to material. We used this platform to test continuous and discontinuous electric read-out. Further studies will be headed using BNNT as a piezoelectric sensor with similar design.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-30**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

술포네이트 폴리스타이렌 아이오노머의 상처 치유에 미치는 아민의 영향

조명근 유정아[1] 김준섭[2,*]

조선대학교 응용화학소재공학과 [1]조선대학교 화학교육과 [2]조선대학교 생명화학고분자공학과

본 연구에서는 종류가 다른 아민으로 중화된 술포네이트 폴리스타이렌 아이오노머의 표면 상처가 다양한 온도에서 어느 정도 치유되는지를 조사하였다. 아이오노머 매트릭스 유리전이온도 근처에서는 표면 상처 치유가 에틸아민으로 중화된 아이오노머의 경우에는 24 시간 뒤에 약 1/2 정도 되었고 옥틸아민으로 중화된 아이오노머의 경우에는 3/4 정도가 되었다. 그리고 매트릭스 유리전이온도 보다 약 20 ℃ 높은 온도에서 열처리하면 에틸아민이나 옥틸아민 으로 중화된 아이오노머의 경우에 치유가 9/10 정도로 거의 비슷했다. 이러한 사실로 보아 옥틸아민으로 중화하는 것이 에틸아민으로 중화하는 것보다 아이오노머의 상처 치유에 더 좋다는 것을 알 수 있었다.

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발표코드: **POLY.P-31**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

pH-Tunable Thermoresponsive PEO-based Functional Polymers with Pendant Amine Groups

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UNIST 화학과 [1]University of California, Santa Barbara, U.S.A

Thermoresponsive polymers exhibiting lower critical solution temperatures (LCSTs) in aqueous solution have garnered considerable attention for the development of smart materials. Herein, we report the synthesis and properties of pH-tunable thermoresponsive poly(ethylene oxide) (PEO)-based functional polymers bearing pendant amine groups with varying cloud points. Well-defined poly(ethylene oxide-co-allyl glycidyl ether) (P(EO-co-AGE)) copolymers were prepared via controlled anionic ring-opening copolymerization of ethylene oxide (EO) with 10 mol % of a functional allyl glycidyl ether (AGE) comonomer. Facile, modular thiol–ene click chemistry was then employed to introduce a library of different aminothiols as side chains to the initial P(EO-co-AGE) copolymer. Depending on the nature of the pendant amine groups (primary amine, dimethylamine, and diethylamine) and the hydrophobicity of the side chains (ethyl, propyl, and hexyl), the cloud points could be tuned from 44–100 °C under different pH conditions. This is the first systematic investigation into the effect of PEO copolymer side chains on cloud point, which opens up the opportunity to make new thermoresponsive polymers for a variety of smart material applications.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-32**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

PMMA 아이오노머의 표면 상처 치유에 미치는 지방산 유도체의 영향

고광환 조명근[1] 유정아[2] 김준섭[3,*]

조선대학교 첨단부품소재공학과 [1]조선대학교 응용화학소재공학과 [2]조선대학교 화학교육과 [3]조선대학교 생명화학고분자공학과

메틸메타크릴레이트(PMMA) 아이오노머의 열에 의한 표면 상처 치유에 지방산 화합물이 어떠한 영향을 미치는지에 대해 현미경을 이용하여 조사하였다. 또한, 결과를 다른 첨가제를 넣은 시료와 비교하였으며, 주사슬의 극성의 영향도 함께 비교하였다. 사슬 길이가 다른 지방산을 상대적으로 작응 양의 이온기를 가지고 있는 PMMANa 아이오노머에 첨가한 경우, 열에 의한 표면 상처 치유 효과는 사슬 길이가 짧은 지방산은 넣은 시료가 가장 좋은 결과를 보여주었으며, 비슷한 이온기의 양을 가지고 있으며 주사슬의 극성이 다른 PSMANa 아이오노머와 비교했을 경우는 주사슬이 비극성인 PSMANa 아이오노머가 더 좋은 표면 상처 치유 효과를 보여주었다. 이러한 결과는 첨가된 지방산 화합물들이 주사슬이 비극성인 아이오노머에 가소제 효과가 더 크게 작용하기 때문인 것 같다.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **POLY.P-33**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

PEG 화합물을 포함한 폴리(스타이렌-co-메타크릴레이트) 아이오노머의 열에 의한 상처 치유 연구

고광환 조명근[1] 유정아[2] 김준섭[3,*]

조선대학교 첨단부품소재공학과 [1]조선대학교 응용화학소재공학과 [2]조선대학교 화학교육과 [3]조선대학교 생명화학고분자공학과

본 연구에서는 다양한 분자량을 가지고 있는 폴리에틸렌글리콜을 포함하고 Na 로 중화된 폴리(스타이렌-co-메타크릴레이트) [PSMANa] 아이오노머의 표면 상처가 열에 의해 어떻게 치유되는지를 조사하였다. PSMANa 아이오노머의 경우 시간이 증가함에 따라 열에 의한 상처 치유 효과가 점진적으로 증가하였다. PEG 를 첨가한 시료의 경우에 분자량이 2000, 4000 인 PEG 를 포함한 시료들은 상처 치유 효과가 비슷하였으며, 분자량이 6000 인 PEG 화합물을 포함한 시료가 분자량이 2000, 4000 인 PEG 를 포함한 시료보다 열에 의한 상처 치유 효과를 잘 보여 주었다. 이러한 결과는 저분자량 화합물인 PEG 가 첨가됨에 따라 자유롭게 움직이는 PEG 사슬로 인해 아이오노머가 멀티플렛을 형성하는데 방해받기 때문인 것 같다.

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장소: 일산 KINTEX
발표코드: **POLY.P-34**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of organic molecular networks with hierarchical pore and its high-efficiency adsorption of carbon dioxide

남준식 박지웅*

GIST 신소재공학부

Urea-based organic molecular networks were synthesized by using cross-linking polymerization of tetrakis (4-aminophenyl) methane and hexamethylene diisocyanate. This study shows that crosslinked urea-network polymer(UN) can be molded into the desired shape with a various length scale of pore diameter. UN was thermally treated at 250~380℃ for thermal rearrange reaction. Rearranged urea-network polymer(RUN) contains a higher volume of micropore and surface area than UN. The resultant hierarchical porous material has excellent carbon dioxide adsorption capacity and selectivity. Furthermore, we are going to discuss how melamine added copolymer affects to thermal treatment condition and carbon dioxide adsorption selectivity.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-35**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

A dramatic upsurge in the diffraction efficiency of the epoxy based azo-polymer using ionic liquid

이상준 김인태*

광운대학교 화학과

In this information age, we have focused on the photosensitive materials for the information storage devices. In order to synthesized the photosensitive azo-polymer and studied the surface relief-grating (SRG) fabrication and real time image recording using diode-pumped solid-state (DPSS) laser of 532 nm, and diffraction efficiency (DE) of polymer using low power DPSS laser at 633 nm. But, the DE of synthesized polymer is low even after 15 min exposure. Hence, to increase the efficiency and reduce the time of DE measurements for synthesized polymer, we have investigated the SRG and DE with combination of azo-polymer and ionic liquids (ILs). We have used various ILs such as 1-methylimidazolium chloride ([Mim]Cl) from imidazolium family IL. Diethylammonium dihydrogen phosphate (DEAP), triethylammonium 4-aminotoluene-3-sulfonic acid (TASA) and tributylmethylammonium methyl sulfate (TBMS) from ammonium family ILs. For the first time, we observed that DE has increased dramatically for DEAP-azo-polymer mixture in 4 min as compared to azo-polymer (alone) and other polymer-IL mixtures. Therefore, DEAP IL can help in increasing the efficiency of DE measurements in less time.

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장소: 일산 KINTEX
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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, characterizaion and properties of new conjugated conducting polymer

한지웅 김인태*

광운대학교 화학과

A newly synthesized conjugated polymer was successfully synthesized using Microwave. This polymer with benzodithiophene derivatives was synthesized by Stille cross-coupling reaction. The structure of polymer was identified by ^{1}H-NMR and UV-Vis spectroscopy. Conductivity of this polymer was measured using conductivity meter. The thermal stability of this polymer was investigated by Thermogravimetric Analysis(TGA) and molecular weights were measured using Gel Permeation Chromatography (GPC).

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장소: 일산 KINTEX
발표코드: **POLY.P-37**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Multilayered structure composites using copper plated oblate ellipsoids for electromagnetic interference shielding application

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anisotropic Cu plated ellipsoids were prepared which had excellent electromagnetic shielding effectiveness of 62.1 - 80.0 dB at a frequency range between 300.0 KHz and 12.0 GHz. . Cu-coated hollow polymer beads were preparedd by electroless plating of copper on the polymer hollow beads. These beads were put into polymer composite through simple compression molding process, which yield 2-dimensional anisotropic shape of filler. The resulting electromagnetic shielding performance were ascribed to a low percolation behavior of the composites and their multilayered structure in the composites.

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장소: 일산 KINTEX
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발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Flame retardancy and mechanical properties of poly(2,6-dimethyl-1,4-phenylene ether) (PPE)/nylon 66 blends prepared by melt extrusion

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The polymer blends with the flame retardancy such as PPE are attracting lots of attention in various fields such as construction materials, automotive interiors, electric and electronic devices etc. In the present study, poly(2,6-dimethyl-1,4-phenylene ether) (PPE)/nylon 66 blends at the ratio of 60/40 were prepared by twin screw extruder at 275 oC. with the compatibilizer and an impact modifier, respectively. Non halogenated flame retardant was used to endow the flame retardancy and well-dispersed flame retardant particles without large agglomerate in the PPE/nylon 66 blends were confirmed through the EDX spectroscopy. For the testing of flame retardancy, UL94V method was carried out and the cone calorimetry was used. The mechanical properties of PPE/nylon 66 blends optimized by each component were deteriorated with increasing the flame retardant loadings. At the result of flame retardany test, HRR (heat release rate) was dropped as well as the maximum peak of the blends were reduced and broadened with increasing FR loadings. In addition, the blends containing ~3 phr flame retardants represented the no grade, while further addition showed V0 grade apparently.

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장소: 일산 KINTEX
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발표분야: 고분자화학
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3D Printed Functional Polymeric Structure with Controlled Surface Area for Adsorption of Heavy Metal Ions

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서강대학교 화학과 [1]서강대학교 화학과 신관우교수님 연구실 [2]서강대학교 화학과 및 바이오융합과정

3D printing which produces objects directly from Computer Aided Designs (CAD) is one of the most versatile and revolutionary technique. 3D printing is a very simple and easy technique to fabricate complex structures which are customized to any personal needs without additional specific tools for the structures. In the meantime, heavy metal pollution has become one of the most serious environmental problems nowadays. Various methods for heavy metal removal including chemical precipitation, ion-exchange, adsorption, membrane filtration and electrochemical methods have their own pros and cons. We fabricated optimized 3D printed polymeric structures for efficient heavy metal removal in the flowing water. These customized polymeric structures are designed to have high surface area coming from specific patterns of structures and modified porous polymeric surfaces. We analyzed the amounts of heavy metal ions in the water are decreased which filtered by these surface area-controlled 3D printed patterns.

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장소: 일산 KINTEX

발표코드: **POLY.P-40**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Hydrophobic Properties of Epoxy-based Composites by Surface Modification of Silica Microparticles

홍준표 노석진[1] 구종민[2,*]

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Outdoor insulation for medium-high voltage require materials with anti-weather properties that are superior to those of other insulating materials such as epoxy resins. Silicone rubbers and nano-fillers are widely used in these applications, but they are weak in physical properties and lack durability. Recently, many studies have reported hydrophobic surfaces using nanostructures. However, these are fabricated synthetic nanostructure surfaces are temporary as the initial hydrophobicity is difficult to maintain over time due to the weak mechanical properties. In this study, we used a commercial cycloaliphatic epoxy resin and modified natural silica fillers surface passivated with organosilane coupling agents.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-41**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

높은 내열성과 유동성을 가지는 폴리카보네이트 공중합체 수지 개발

정승필 허성현 신경무*

(주)삼양사 화학연구소

폴리카보네이트 수지는 내열성, 기계적 물성 (특히, 충격강도) 및 투명성이 우수하여 전기부품, 기계부품 및 산업용 수지로서 광범위하게 사용되고 있다. 특히 전기전자 분야 중에서 열이 많이 발산되는 TV 하우징, 컴퓨터 모니터 하우징, 복사기, 프린터, 노트북 배터리, 리튬 전지의 케이스 재료 등으로 폴리카보네이트 수지를 사용하는 경우에는 기계적 물성뿐 만 아니라 우수한 내열성이 요구된다. 삼양사에서 개발한 고내열 폴리카보네이트 제조기술은 폴리에스테르 화합물과 폴리카보네이트 블록 공중합체를 제조하여 높은 내열성 및 유동성을 가진다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-42**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of Eco-Friendly Flame-Retardant Polycarbonate

박정업 최진식 신경무*

(주)삼양사 화학연구소

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 분지상 폴리실록산-폴리카보네이트 블록 공중합체를 제조하여, 난연제를 사용하지 않고도 난연성을 충분히 발휘하며, 동시에 우수한 투명성을 만족시킨다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-43**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Polyethylene Glycol Substituted Oxidized Carbon Nitride for F-18 Labeling Polymer

변강록 **Mudumala Veeranarayana Reddy** 우상식 한혜지 김동욱*

인하대학교 화학과

Polyethylene glycol substituted oxidized carbon nitride (OCN-PEG-OH) has numerous benefits due to the special structure. Two-dimensional (2D) Oxidized Carbon Nitride (OCN) which is a basic structure of the OCN-PEG-OH has different chemical, physical, morphological properties compared with 3D allotropes. So OCN-PEG-OH also has high surface area, water-dispersible and law toxic nature. Moreover, poly ethylene glycol (PEG) substituted to nitrogen atoms of OCN-PEG-OH nano sheet structure has terminal hydroxyl group which is easily mesylated and then labeled with radioactive 18-F. Therefore OCN-PEG-OH is the first polymer directly labeling with 18-F, and is available to living cells due to the chemical stability and low toxicity.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **POLY.P-44**

발표분야: 고분자화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Polymorphic Superstructures of Pyrene-Based Asymmetric Supramolecule

박민욱 정광운[1,*]

전북대학교 고분자나노공학과 [1]전북대학교 고분자.나노 공학과

In order to grasp the kinetically controlled polymorphic superstructures from asymmetric supramolecules, a pyrene-attached asymmetric supramolecule (abbreviated as Py3M) was newly synthesized. Superstructures of Py3M exhibited the monotropic phase transition between a stable crystalline phase (K1) and a metastable crystalline phase (K2). Py3M formed two synclinically tilted crystalline superstructures: the 6.75 nm and 4.30 nm periodicities of layered structures for K1 and K2 phases, respectively. The stable K1 phase and metastable K2 were predominantly induced by the π-π interactions and hydrogen-bonds. UV-Vis and PL experiments indicated that the photo-physical properties of Py3M were directly related with their molecular packing superstructures. This work was mainly supported by Mid-Career Researcher Program (2016R1A2B2011041), BK21 Plus program, Korea, and BRL (2015042417) of Korea.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-45**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Enhanced Photonic Property of Quasi-amorphous Photonic Solution by Introducing Imaginary Part of Refractive Index

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한양대학교 화학과 [1]한양대학교 자연과학대학 화학과

General photonic crystals are made up materials that have different real part of refractive index and until now, imaginary part of refractive index in photonic crystals is not considered. So, we investigated how absorbance affect to reflectance of photonic crystals and use polydopamine (PDA) nanoparticles as absorbing material. When PDA put into SiO2 quasi-amorphous photonic solution (QAPS), PDA/SiO2 QAPS shows high contrast photonic color and enhanced reflectance. Also, when dye trapped polystyrene (PS) nanoparticles are added in QAPS, novel phenomena occurred. Only when photonic bandgap region matched with absorbance band of dye, reflectance of QAPS enhanced. Otherwise reflectance intensity not changed. This result show interplay between absorption and reflectance and considerably encourage in field of optics using photonic crystals.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-46**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Preparation of Dual Color Electrochromic devices with Poly(3,4-propylenedioxythiphene) derivatives

허영환 나종범 김영훈 이우재 한민수 김은경*

연세대학교 화공생명공학과

Conjugated polymers (CPs) show reversible electrochemical optical changes with a high coloration efficiency, which can be applied for external light control such as smart windows, light modulators, and displays. Among the CPs, poly(3,4-propylenedioxythiphene) derivatives(PRs) have large color tunability. Using red and blue electrochromic PRs, a dual color electrochromic polymer device was prepared. Mechanism for the dual color switching and the effect of charge balancing on the electrochromic contrast of the dual color electrochromic device will be presented.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **POLY.P-47**
발표분야: 고분자화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Room-Temperature Synthesis of Bright Fluorescent Thermal Stable and Color Tunable Formamidinium Lead Halide Perovskites Nanocrystals: A Better Candidate for Optoelectronic devices

NGUYEN MINH DUONG 강영종[1,*]

한양대학교 화학과 [1]한양대학교 자연과학대학 화학과

Perovskite lead halide nanocrystals have been researched intensively within the last few years due to the fascinating optical properties, such as, high photoluminescence quantum yield (PLQY) reach almost 100%, narrow full-width half maximum (FWHM) less than 30nm, color tunable cover the whole visible spectra, low cost and possible solution process, potential to be newcomer class in light emitting diodes (LEDs) devices. Perovskite lead halide nanocrystals has the common formula APbX3 (X=Cl, Br and I), whereas A can be only three cations, methylammonium (MA), cesium (Cs) and formamidinium (FA) to maintain the crystal structure of perovskite materials. For last two years, MAPbX3 and CsPbX3 have been synthesized successful and proved their promise as a possible material to be commercialized in LED devices. However, it still challenges and lacks a method to synthesize the last perovskites family member FAPbX3 with the color tunable. Although, it is estimated that FAPbX3 is a better material compare with MAPbX3, according to the smaller band gap improved light-harvesting, and higher thermal stability in solar cell. In this work, we first time provide a new precursor materials to synthesize successful FAPbX3 nanocrystals at room temperature, with color tunable up to infrared region (408-784nm), narrow FWHM (18-48nm), high PLQY up to 75% and higher thermal stability compare with conventional MAPbX3 nanocrystals. Our work will open a new class in perovskite nanocrystals, providing a promising candidate for optoelectronic devices.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-1**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The carbon black surface treatments and their using black colour materials

박수열* 이병민

한국화학연구원 계면화학공정연구센터

Carbon Black(CB) is obtained from the partial combustion or thermal decomposition of hydrocarbons. Its primary particles exhibit a spherical shape which form aggregates. The aggregates are further agglomerate because of strong van der Waals forces among the surface of the CB nano particles. These material depends on its dispersion, however, it exhibits a strong tendency to agglomerate, and the preparation of a stable dispersion of the material in organic solvents or in polar solvents such as water. This experiment describes the results of reacting dialkylamines with carbon black that had been oxidized in nitric acid for varying times. Reacting alkylamine groups with oxidized carbon black could introduce several amino functions for each carboxyl group consumed. In this way the total amount of available surface-bound functional groups could be increased. Therefore, the dispersions of the modified CB was stable in organic solvents and water base.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **IND.P-2**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

전단결합 강도가 향상된 치과용 시멘트 재료 연구

김득현 이민제 성아영*

대구가톨릭대학교 안경광학과

치과용 시멘트는 치아 수복물 또는 교정창치의 고정 등의 역할을 하는 치과치료 재료로 구강의 정상적인 피부외의 생체조직과 접촉하여 사용하는 재료이며, 치과용 세라믹의 접착은 최종 단계인 동시에 치과적 치료의 성공을 결정하는 매우 중요한 단계로서 접착단계에서 치과용 시멘트가 사용된다. 시멘트는 삭제된 치아와 수복물 사이의 유지력을 제공하는 접착제의 기능을 하고 동시에 형성된 와동을 영구적 또는 임시적으로 충전하는 수복재로서 사용된다. 본 실험은 치과용 시멘트 중합을 위해 Bis-GMA, HEMA, TEGDMA 등을 사용하여 혼합물을 제조하였다. 또한 광 개시제로 camphoroquinone 을 사용하였으며, 접합강도를 증가시키기 위해 기능성 첨가제를 다양한 비율로 혼합하여 실험하였다. 또한 460 nm 파장의 영역대에서 30 초 동안 광중합 하여 레진시멘트를 제조하였다. 각 시료의 광중합 결과, 모든 조합에서 30 초 이내에 단단한 레진시멘트가 생성되었으며 독성평가 결과 모든 조합에서 적합 하였다. 또한 접합 후 각 시편의 전단결합 강도를 측정한 결과, 5.75~8.28 Mpa 로 나타나 고강도 치과용 레진시멘트로서 활용 가능할 것으로 판단된다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-3**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photophysical Properties of Isomeric Blue Phosphorescent Ir(III) Complexes with Cyclometalated Carbene Ligands

윤보선 강상욱 손호진*

고려대학교 신소재화학과

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. We report a study of the synthesis and photophysical properties of cyclometalated iridium complexes, some of which emit in the blue part of the spectrum, with N-heterocyclic carbene ligands: $[\mathrm{Ir(dmfmi)_3}]$, Iridium, tris[(9,9-dimethyl-9*H*-fluorene-3,2-diyl)(3-methyl-1*H*-imidazol-1-yl-2(3*H*)-ylidene)]. Imidazolyl-carbene ligand has a stronger trans influence than $(\mathrm{C{\wedge}N})$ ligand and, thus, imparts a greater ligand field strength. Both *mer*-$\mathrm{Ir(dmfmi)_3}$ and *fac*-$\mathrm{Ir(dmfmi)_3}$ complexes display strong metal-to-ligand-charge-transfer absorption transitions in the UV (λ = 270-370 nm) and phosphorescene in the blue region ($E_{0\text{-}0}$ = 455 nm, 467 nm) at room temperature. The meridional and facial isomers show different spectroscopic properties each other and meridional isomers leads to the observation that they are easier to oxidize, exhibit red-shifted emission, and have lower quantum efficiencies than their facial isomers.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-4**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoinduced Electron Transfer and Intramolecular Charge Transfer Processes: The Influence of π-Conjugation on Competitive Pathways

김태현 강상욱 손호진*

고려대학교 신소재화학과

In order to explain 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 Dδ+–π–Aδ- 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 (Δμ = 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: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-5**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Iridium(III) Complexes Containing N-heterocyclic Carbene Ligands for Blue Phosphorescent OLEDs

김종훈 강상욱 손호진*

고려대학교 신소재화학과

The combination of both very high brightness and deep blue emission from phosphorescent organic light-emitting diodes (PHOLED) is required for display and lighting applications, yet so far development of high performance blue phosphorescent OLEDs and related materials is still a challenging issue. Blue phosphorescent OLEDs are the most difficult to achieve high efficiency among three primary colors due to its limitation on the selection of materials satisfying the requirements of host materials and neighboring charge transporting materials with higher triplet energy than that of the blue emitter for efficient triplet confinement within emitter and 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. Our results represent an advance in blue-emitting PHOLED architectures and materials combinations that meet the requirements of many critical illumination applications.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **IND.P-6**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Series of Sulfonyl-Substituted Heteroleptic Iridium(III) Complexes with Tunable Emission Wavelength and Excited State Properties: Structures, Theoretical Calculations, and Photophysical and Electrochemical Properties

김진형 강상욱 손호진*

고려대학교 신소재화학과

Development of blue phosphorescent emitter is one of the key challenges in the field of organic light-emitting diodes (OLEDs). In this study, we report on the synthesis and photopysical characterization of heteroleptic cyclometalated sulfonyl-substitued Iridium(III) complexes with ancillary ligands, such as the $Ir(C\^{}N)_2$(ancillary ligand), (C^N = 3-(pyridin-2-yl)benzene-1-sulfonyl fluoride (SO_2F), 2-(3-(trifluoromethylsulfonyl)phenyl)pyridine (SO_2CF_3); ancillary ligand = acetylacetone (acac), borate (bor) and picolinate (pic)). A systematic blue-shift on the emission spectra is observed on the variation of ancillary ligand from acac (λ_{max} = 490 nm) to bor (λ_{max} = 460 nm). Density-functional theory (DFT) calculations on the HOMOs and LUMOs for this series show a trend similar to those observed from photophysical and electrochemical analyses. The sulfonyl-substituted Iridium complexes having bor moiety as ancillary group ($Ir(SO_2F)_2$(bor) and $Ir(SO_2CF_3)_2$(bor)) were shown to be a potential blue-emitting material, exhibiting a maximum efficiency of 2850 cd/m^2 at 7.8 V with 8.1 cd/A in a multilayered device structure of ITO/PEDOT:PSS/PVK:OXD-7(35%):Ir Complex(15%)/TPBi/LiF/Al.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-7**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optical Properties of Heteroleptic Ir complexes: Ligand-to- ligand Charge Transfer of Metal Complexes

박재현 강상욱 손호진*

고려대학교 신소재화학과

Through the synthesis that two types of heteroleptic Ir complexes ($Ir(dfppy)_2(tpphz)$) and ($Ir(dfppy)_2(dpq)$), we found the electronic spectra of metal complexes which contain a reducing and an oxidizing ligand (L_{red}–M–L_{ox}) are characterized by ligand-to-ligand charge transfer (LLCT) absorptions. Because of the tpphz and dpq ligands π-conjugation are longer than dfppy, ligand-centered(LC) and metal-to-ligand charge transfer(MLCT) states are low. The LLCT from dfppy to tpphz (or dpq) was investigated femtosecond transient absorption (TA) spectroscopy in excitation of dfppy. As the LLCT process have been changed for the TA bands involved with increased of the MLCT states of tpphz or dpq ligand and those of dfppy decreased, LC/MLCT state of dfppy has shown 480 nm. According to the MLCT emission of $Ir(ppy)_2$(tpp hz) showed strong temperature dependence, since the LLCT process has a significant energy barrier. The LLCT process showed 17 ps for $Ir(dfppy)_2(tpphz)$ and 5 ps for $Ir(dfppy)_2(dpq)$ time constants. As the emission of $Ir(dfppy)_2(dpq)$ influenced weakly the temperature, we know LLCT process has a smaller barrier. Moreover, the anomalous rigidochromism and photodynamic behaviours can be explained in terms of the barrier between cyclometalating and ancillary ligands.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-8**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Emissive Cyclometalated Ir(III) Complexes: Synthesis, Characterization, Photophysical properties and DFT calculations

손미랑 김철훈 강상욱 손호진*

고려대학교 신소재화학과

A series of homoleptic cyclometalated iridium(III) complexes having phenylimidazole ligands were prepared to study emission properties pertinent to the phenylimidazole ligands. Ir complexes bore tris-C^N-chelated hexa-coordinated metal centers with exclusive *meridional* conformation: products were **Ir(dmp)$_3$, Ir(dmp-CH$_3$)$_3$, Ir(dmp-F)$_3$** and **Ir(dmp-CF$_3$)$_3$** in which phenylimidazole ligands varied in the *para*-position of the phenyl group with H, CH_3, F and CF_3 groups. Systematic emission color change was apparent within the context of electron withdrawing substituents on going from phenyl to trifluoromethyl group. Density-functional theory (DFT) calculations estimated the emissive triplet states that were closely examined by photodynamic studies. Due to the bulky planar nature of the ligand, ^{3}MLCT was a dominant emissive origin and this ensured stability of the complexes accordingly. Device fabrication led to potency of this bulky planar ligand and device performance and ligand structure relationship will be discussed.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-9**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dendrimers Containing Organometallic Complex Designed for Functions: Photoinduced Electron and Energy Transfer

차현욱 김철훈 강상욱 손호진*

고려대학교 신소재화학과

Luminescent dendrimers have largely been used as ligands for transition-metal. The resulting properties are (i) shielded excited states from quenching processes, (ii) light harvesting, (iii) conversion of incident UV light into visible or infrared emission, and (iv) metal ion sensing with signal amplification. We prepared dendrimers of heteroleptic iridium(III) complexes, Cz_n-Ir(dpq) (G_n, n = 0–2), which have the carbazole-functionalized dendron. Upon exciting the carbazole chromophore of G1 and G2 at 309 nm both the carbazole fluorescence and the MLCT emission were very weak at room temperature. These observations demonstrate that both the excited singlet state of carbazole and the triplet MLCT state of the Ir(dpq) core are efficiently quenched in the dendrimers. Since the apparent quenching of either carbazole fluorescence or MLCT emission observed at room temperature does not occur at 77 K, the temperature-dependent emission behavior of G1 and G2 for both the carbazole fluorescence and the MLCT phosphorescence was attributed to the participation of activated processes, that is, electron transfer from excited-singlet carbazole to the Ir(dpq) core. On the other hand, the increase in phosphorescence efficiency was estimated by the energy transfer mechanism for Ir(pic-Cz_n) (G_n, n = 0–3). Selective excitation of the Cz_n units of G1–G3 resulted in >90% quenching of the Cz fluorescence accompanied by the growth of phosphorescence from the Ir(pic) core as a consequence of energy transfer from the excited-singlet Cz_n chromophore to the core. Finally, the light-harvesting efficiencies for dendrimers were determined to be 162–334%.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **IND.P-10**

발표분야: 공업화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

회수 TNT의 특성 평가 및 규격 분석 연구

추초롱 김진석[1,*]

국방과학연구소 4본부 [1]국방과학연구소 4본부 2부

사용수명이 종료된 포발사탄으로부터 TNT 가 배출되어 나오고 있다. 이러한 TNT 는 50 년 정도의 저장 및 장기간 운용 기간 중 다양한 환경 하에서 보관되어 왔으므로, 각종탄으로부터 용출된 TNT 중에는 화학적인 변화를 포함하는 불량 TNT 도 존재할 수 있다. 이러한 불량 TNT 를 사용할 경우, 포발사 시에 인가되는 높은 순간압력에 의해 포신내에서 폭발하여 인명피해를 입을 수 있으므로 엄격한 평가가 이루어져야 한다. 본 연구에서는 이러한 회수 TNT 의 사용방안을 수립하기 위하여 비군사화 사업장에서 시료를 채취하고, 장기저장에 따른 TNT 의 이화학적 특성변화를 분석하였다. 이를 위해 미량분석에 주로 사용되는 high performance liquid chromatography(HPLC)분석을 시행했다. 그리고 이 결과를 바탕으로 회수 TNT 를 평가하고 향후 회수 TNT 사용방안 수립시 활용하고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-11**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile ion transport in smectic-ordered ionogel

박서경 이제승*

경희대학교 화학과

Self-assembled ionic liquid crystals composed of ionic liquid and lithium salt have been prepared and their ion transport behavior were investigated. The ionic mixtures were prepared by mixing an imidazolium based-ionic liquid containing ether-functionalized anion with the lithium salt which self-assembled into the smectic-ordered structure via Coulombic interactions. The prepared ionogels showed solid-like viscoelasticity behavior. Unexpectedly, the ionogels exhibited higher ionic conductivity than the pure ionic liquid despite of their solid-like viscoelasticity. The structural features of ionogels were characterized by optical birefringence, SAXS and NMR spectroscopy.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **IND.P-12**
발표분야: 공업화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Preparation of ammonium carbonate solution by catalytic hydrolysis of urea

박서경 이지현 이제승*

경희대학교 화학과

The solutions of ammonium carbonate and urea have been widely used to reduce nitrogen oxides (NO_x) emissions from combustion of fossil fuels and diesel engine. Industrially, ammonium carbonate easily has been produced by reaction of ammonia and carbon dioxide (CO_2). However, this method has drawbacks such as the toxicity of ammonia and producing water-insoluble ammonium bicarbonate as a by-product. Herein, we will discuss the simple and efficient method for preparing ammonia carbonate-urea solution using urea as a raw material.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-48**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Control of Cellular Proliferation on Nanostructures of Hexagonally Close-Packed Silica Bead Arrays

박이슬 김규리[1] 이진석[1,*]

숙명여자대학교 화학과 [1]숙명여자대학교 화학과

Biochemical cues ignore cellular microenvironments such as cell to cell interaction and extracellular matrix (ECM). In recent year, various studies have shown that nanotopological cues regulate cell behavior such as cell adhesion, cell proliferation, migration, polarity, and differentiation. Although many previous studies have investigated cell behavior using various topographical cues, the results have meant topographical confinement by nanostructured architecture. That is, overall control of cellular response is carried out by cells isolation in the structure through geometry, and is not affected by surface topography. In previous study, we described that hippocampal neuron on silica beads bigger than 200 nm in diameter accelerated neurite outgrowth and formed the lamellipodia and filopodia.In this study, we investigated the effects of the hexagonally close-packed silica bead arrays on cellular behavior, especially adhesion and proliferation. The silica beads were synthesized by stöber method by controlling the amount of reagents or injection rates. In addition, the hexagonally close-packed silica bead arrays can be achieved by rubbing method, which is simple and fast to obtain monolayer of silica beads. The different size of silica beads were examined to figure out the nanotopological effect on the cellular behavior, which are range of 300 nm to 1800 nm. The silica beads arrays classified by two groups, such as Group-I and Group-II, of nanotopological effect along with cell adhesion and morphology. The Group-II surface was long distance between contact points, resulting in increase of tension to cells. The proliferation of cells increased by decreasing cell adhesion and spreading behavior.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-49**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Bioinspired Silicification on the Nanostructured Surface by Local Liquid Phase Deposition

박이슬 김규리 이진석*

숙명여자대학교 화학과

Organisms can biosynthesize hierarchically patterned three-dimensional (3D) biominerals, called as biomineralization, such as calcium carbonate, calcium phosphate, and silica. The structural hierarchy in biominerals attributes strengths and stiffness, leading to protect themselves from natural environment. Especially, the process for production of silica into the living organism is known as biosilcification, which are often discovered in the diatom. Diatoms are complex and elaborated nano- and microstructured materials, whose architectures have numerous nanoscale pores with high porosity and high mechanical stability.In this work, we explored the silicification on the arranged nanoscale-scaffold surface with porous structures, to mimic 3D hierarchical structures of diatoms by local liquid phase deposition. The energy and local concentration of silicic acid on the nanostructured surface are different; therefore, it is important to investigate the liquid phase deposition on the nanostructure with diverse conditions to mimic and understand the mechanism of bioinspired morphogenesis. The different amount of water in LPD solution and reaction temperatures were used to investigate the effect of diverse environment because the biosilicification of diatoms occurs in the various surrounding environment such as concentration, temperature, and pressures. In addition, the silicification on the nanostructured surface deposited at the pinholes among the beads due to local high concentration. Furthermore, the pore arrangement and directions with 3D hierarchical structures were realized by patterned silica bead arrays and binary monolayers of different sized beads with varying the LPD conditions.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-50**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Sequential Growth of Hybrid Organic-Inorganic Zincone Film on Nanostructures by Molecular Layer Deposition

최의진 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, nanobead, nanowire array and so on. In this study, we fabricated organic-inorganic zincone polymeric films on surfaces with various curvatures through coupling reactions between diethyl zinc (DEZ) and diol with triple bonds as inorganic and organic precursors, respectively, by molecular layer deposition. Using ellipsometry and transmission electron microscope (TEM), we confirmed the different growth rate of the films on nanostructure versus number of MLD cycles at all same temperature. The mass gains in zincone films grown with varying doses of DEZ and organic diol were identified using in situ quartz crystal microbalance (QCM) technique. And, surface potential of zincone films according to the curvature surfaces was investigated by ex situ analysis scanning kelvin probe microscopy (SKPM). Furthermore, all molecular geometries on surfaces with various curvatures 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.[5] Y.-S. Park, H. Kim, B. Cho, C. Lee, S.-E. Choi, M. M. Sung, J. S. Lee*, ACS Applied Materials & Interfaces, 2016, 8 (27), 17489–17498.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-51**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Continuous $Mo_xW_{1-x}Se_2$ Film with Tunable Band Gap via Metal-Organic Chemical Vapor Deposition

이유빈 이진석*

숙명여자대학교 화학과

Study of transition metal dichalcogenides (TMDC) are interested due to their optical, electronic properties. Synthesis of heterostucture TMDC like $Mo_xW_{1-x}S_2$ has researched variously. But, one of the spotlighted synthesis techniques, metal organic chemical vapor deposition (MOCVD) for synthesis TMDC materials and TMDC alloy films has not been reported yet.Here, we present the report of synthesis continuous $Mo_xW_{1-x}Se_2$ films via metal organic chemical vapor deposition method using molybdenum hexacarbonyl ($Mo(CO)_6$), tungsten hexacarbonyl ($W(CO)_6$) and dimethyl selenide ($Se(CH_4)_2$) on silicon oxide wafer and characterized by atomic force microscopy (AFM). We observed two peaks of A_{1g} mode, main Raman modes of $MoSe_2$ and WSe_2, using micro-Raman spectroscopy and show tunable optical band gaps by photoluminescence measurements that they are detected different intensity and position, respectively. This study will attract us to discuss tunable band gap engineering applications that we have enlightened with continuous TMDC alloy.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-52**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Macrocyclic Copper(II) Complex with 1,2,4,5-Benzenetetracarboxylate Ligation

김태영 김주창*

부경대학교 화학과

Copper(II) complex, $\{[Cu(L)(H_2O)_2][Cu_2(L)_2(\mu\text{-btc})]\cdot 2ClO_4\cdot 6H_2O\cdot 1.454CH_3CN$ (1) (L = tetraazamacrocycle, btc = 1,2,4,5-benzenetetracarboxylate ion) was prepared by the reaction of $[Cu(L)](ClO_4)_2$ and $btcH_4$ in $DMF/H_2O/CH_3CN/NEt_3$. 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, two different copper(II) coordination geometries, a five-coordinate square pyramid as well as an axially elongated six-coordinate octahedron, are observed. The btc ligand bridges two copper(II) macrocycles to form a dimer where all the hydrogen atoms of $btcH_4$ were deprotonated, forming a complex dianion. Additional copper(II) macrocycle involves in (1) in which two aqua ligands interact with central metal ion weakly, resulting in the formation of complex dication. Thus, the whole complex (1) is charge balanced. Details of the structural properties will be discussed in this presentation.

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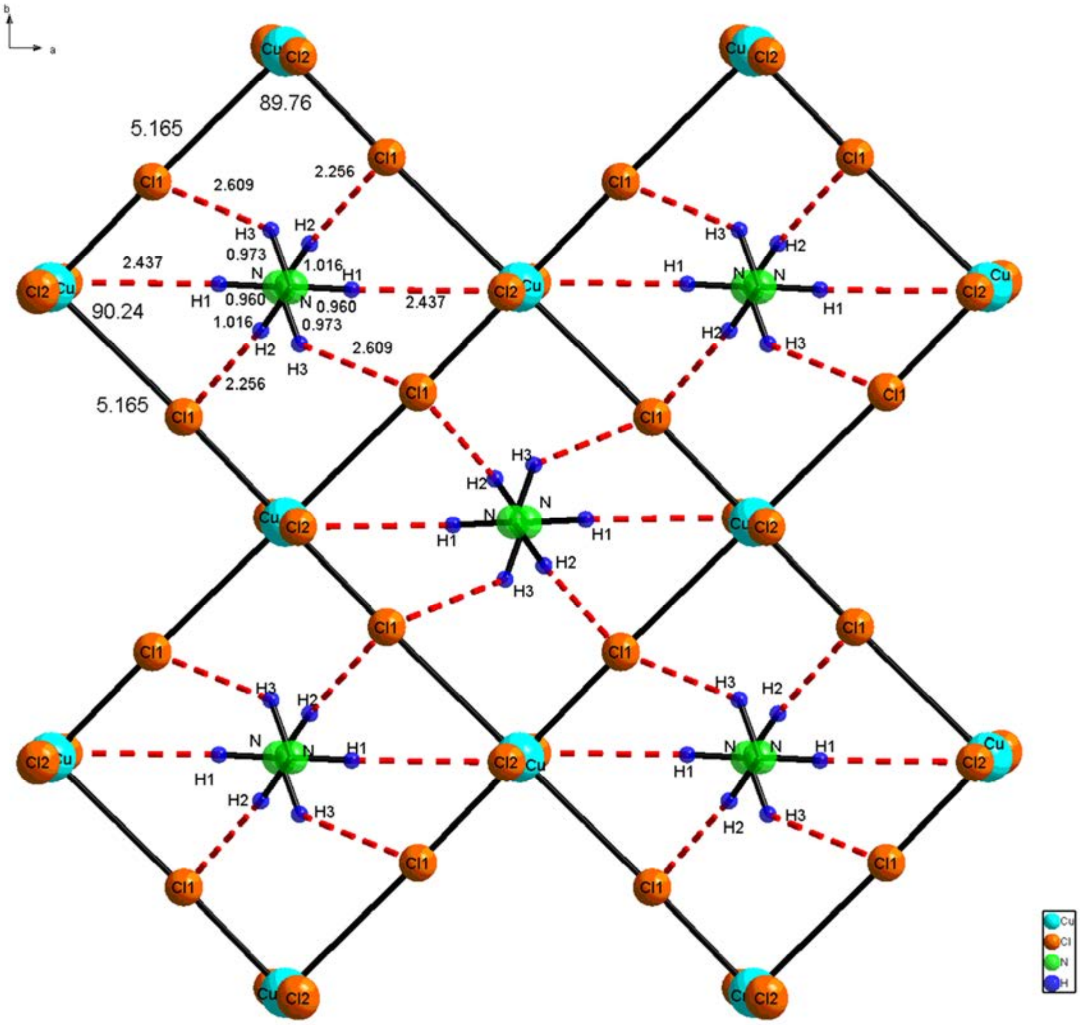
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-53**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Inorganic-organic hybrid perovskite : Crystal structure and phase transitions through crystallographic group-subgroup relations

박가람 오인환[1,*] Martin Meven[2] Gernot Heger[2] 홍창섭

고려대학교 화학과 [1]한국원자력연구소 중성자과학연구부 [2]RWTH Aachen, Germany

$(C_6H_5CH_2CH_2NH_3)_2CuCl_4$ (Cu-PEA) belongs to the layered inorganic-organic K_2NiF_4 perovskite type of general formula A_2 MX_4 , where A = organic cation, M = divalent metal, X = halides. These systems attract special interest owing to their low-dimensional magnetic characteristics. To investigate the effects of the interlayer spacing on the magnetic behavior, various hybrid systems have been developed. In this work, we will present a crystal structure, hydrogen bonds using neutron single crystal diffraction and phase transitions with group-subgroup relations.


b
a
Cu
Cl2
89.76
5.165
Cl1
2.609
2.256
H3
H2
0.973
1.016
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N
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0.960
90.24
1.016
0.960
0.973
2.437
2.609
2.256
5.165
Cu
Cl
N
H

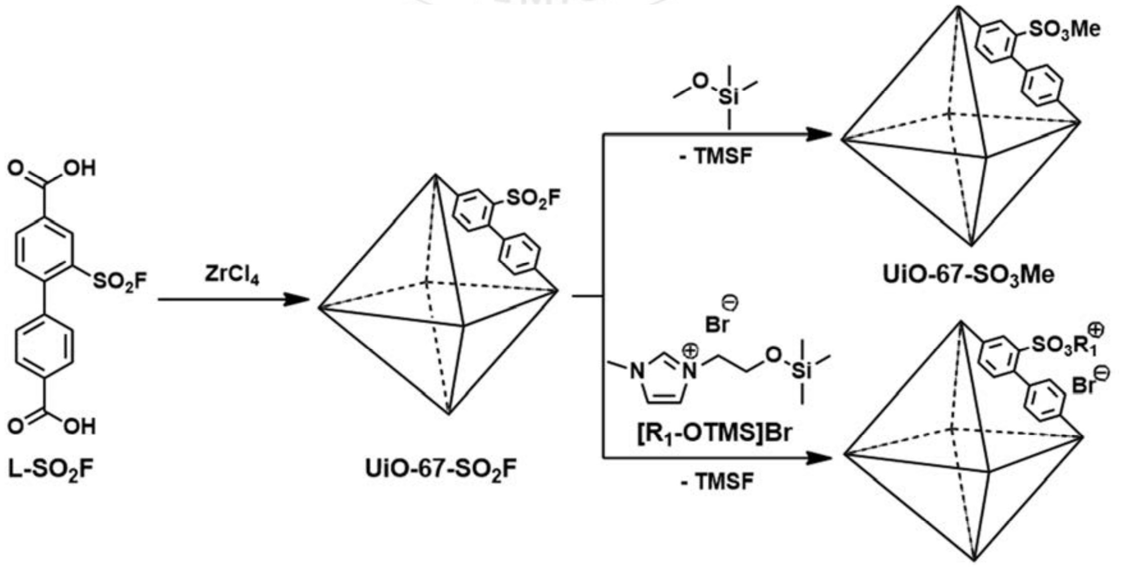
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-54**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

SuFEx-based Post-synthetic Modification of UiO-67

박승재 김기문 이은성*

POSTECH 화학과

Metal-organic frameworks (MOFs) are representative robust and porous crystalline materials consisting of metal and organic linkers. With their interesting properties, MOFs are explored for gas separation, adsorption and catalysis. Various post-synthetic modification (PSM) strategies have been reported to modify the intrinsic properties of MOFs and to enhance the performance in applications. Typically, modification of the organic ligands is the first option for PSM, followed by the exchange of the metal ions. Herein, a new type of click reaction, sulfur(VI) fluoride exchange (SuFEx),[1] has been utilized to prepare two post-synthetic modified (PSM) UiO-67 series, whose single-crystal-to-crystal transformations of the click reaction were confirmed by X-ray single crystal analysis. This SuFEx method will provide versatile tools for introducing new functionality inside MOFs



일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-55**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A highly selective turn-on chemosensor for Zn^{2+} in aqueous media and living cells

김 철* 정재민[1] 황수미[1] 조한나[1]

서울과학기술대학교 정밀화학과 친환경소재제품센터 [1]서울과학기술대학교 정밀화학과

A new simple quinoline-based chemosensor 1 was synthesized for Zn^{2+}. 1 showed the selective fluorescence enhancement in the presence of Zn^{2+} with a 1:1 stoichiometry in a near-perfect aqueous solution (bis-tris buffer:DMSO = 999:1), which was reversible with the addition of ethylenediaminetetraacetic acid (EDTA). The detection limit (0.6 μM) of 1 for Zn^{2+} was much lower than World Health Organization guideline (76 μM) in drinking water. 1 was successfully applied to quantify and image Zn^{2+} in water samples, test kit and living cells. The sensing mechanism of Zn^{2+} by 1 via the intramolecular charge transfer was explained by theoretical calculations.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-56**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A colorimetric and fluorescent chemosensor for the selective detection of Cu^{2+} and Zn^{2+} ions

김민선 양민욱 김 철[1,*]

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A new bi-functional chemosensor 1 based on 3,5-dichlorosalicylaldehyde and 2-(methylthio)aniline has been synthesized. It can detect Cu^{2+} with a color change from pale yellow to dark yellow in aqueous solution. The selective mechanism of 1 for Cu^{2+} was proposed to be the enhancement of the intramolecular charge transfer (ICT) band, which was explained by theoretical calculations. The sensor 1 could be used to detect and quantify Cu^{2+} in water samples. In addition, the sensor 1 displayed “turn-on” fluorescence response only to Zn^{2+}, based on an effect of chelation-enhanced fluorescence (CHEF). Therefore, 1 can serve as a 'single sensor for two different targets' with dual modes.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-57**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A novel colorimetric chemosensor for detection of Co^{2+} and S^{2-} in an aqueous environment

장효정 김 철[1,*] 윤동주

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A novel multifunctional and highly selective chemosensor 1, N 2-(bis(pyridin-2-ylmethyl)amino)-N-(2-((2,4-dinitrophenyl)amino)phenyl)acetamide, for Co^{2+} and S^{2-} was designed and synthesized. Sensor 1 showed a selective colorimetric sensing ability for cobalt ion by changing color from pale yellow to light green in a near perfect aqueous solution. The detection limit (0.99 M) of 1 for Co^{2+} was lower than the Environmental Protection Agency (EPA) guideline (1.7 μM) for drinking water. The sensor 1 could be used to quantify Co^{2+} in water samples. Moreover, sensor 1 detected S^{2-} selectively, which induced an obvious color change from pale yellow to pink over most other competitive anions in aqueous solution. The sensing mechanism of Co^{2+} by 1 was proposed to be a ligand-to-metal charge-transfer (LMCT) with the experimental results and theoretical calculations, and that of S^{2-} by 1 proposed to be a deprotonation process. Therefore, this sensor 1 could be used as a practical system for monitoring both Co^{2+} and S^{2-} in an aqueous environment.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-58**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A novel colorimetric chemosensor for the sequential detection of Ni^{2+} and CN^{-} in aqueous solution

강지혜 김 철[1,*] 김아란

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A new colorimetric chemosensor 1 for the sequential detection of Ni^{2+} and CN^{-} was designed and synthesized. The presence of Ni^{2+} led to a distinct naked-eye color change from colorless to yellow in a near-perfect aqueous solution. To examine the binding mechanism of 1 with Ni^{2+}, UV-vis spectroscopy, ESI-mass spectrometry analysis and DFT calculations were conducted. The detection limit of 1 for Ni^{2+} was down to nanomolar concentration (57 nM). Also, the sensing ability of 1 for Ni^{2+} was successfully carried out in real water samples (tap, drinking and sewage water). Moreover, the resulting 1-Ni^{2+} complex acted as an efficient colorimetric chemosensor for CN^{-} via a color change from yellow to colorless. Therefore, chemosensor 1 can be employed as a practical colorimetric chemosensor for detecting of both Ni^{2+} and CN^{-}.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-59**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and their Electrochemical Properties of 1,1-Diisopropyl(or 1,1-Diphenyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)siloles

조윤호 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

1,1-Diisopropyl(or 1,1-Diphenyl)-3,4-diphenyl-2,5-bis(trimethylsilyl)siloles were prepared by the intramolecular reductive cyclizations of diisopropyl(or diphenyl)bis(phenylethynyl)silanes with treatment of 4.5 mol lithium naphthalenide and followed by 4 mol chlorotrimethylsilane solution in THF. After the reaction was finished, the naphthalene was removed via naphthalene sublimation apparatus, and the crude product was purified by recrystallization. The obtained materials are soluble in usual organic solvents such as THF and $CHCl_3$. The prepared materials were characterized by NMR, and IR spectroscopies. We also studied the electronic properties of the prepared silole derivatives by UV-vis absorption, excitation and fluorescence emission spectroscopic methods, in particular. In order to study the electrochemical properties of the synthesized materials, we also prepared a composite of the obtained carbosilanes with silicon nano powder, and examined the electrochemical properties.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-60**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Electronic Property of 3,4-Diphenyl-1,1-diethyl or dihexyl-2,5-dibromosilole

박지영 박영태[1,*]

계명대학교 화학과 [1]계명대학교 자연과학대학 화학과

Diethyl or dihexylbis(phenylethynyl)silane as precursor were prepared by reactions of dichlorodiethyl or dihexylsilane with of phenylacetylene treated with *n*-butyllithium in situ.2,5-Dibromo-1,1-diethyl or dihexyl-3,4-diphenylsilole as monomers were prepared by the intramolecular reductive cyclizations of diethyl or dihexylbis(phenylethynyl)silane with treatments of lithium naphthalenide and followed by reaction with anhydrous $ZnCl_2$ and N-bromosuccinimide in situ.The obtained silole 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 and fluorescence emission spectroscopic methods along with electrochemical property, in particular.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-61**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, characterization, and catalytic activities of nickel(II) monoamido-tetradentate complex: Evidence for Ni^{III}-Oxo and Ni^{IV}-Oxo species

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A new mononuclear nickel(II) complex, [Ni(II)(dpaq)Cl] (1), containing a tetradentate monoamido ligand, dpaq (dpaq=2-(bis(pyridin-2-ylmethyl)amino)-N-(quinolin-8-yl)acetamide), has been synthesized and characterized by IR, elemental analysis, and UV-visible spectroscopy. The structure of the nickel complex has been determined by X-ray crystallography. This nonheme Ni^{II} complex 1 catalyzed epoxidation reaction of a wide range of olefins with *meta*-chloroperoxybenzoic acid (MCPBA) under mild conditions. Olefin epoxidation by this catalytic system has been proposed to involve a new reactive Ni^{IV}-Oxo (4) species, based on the evidence from PPAA (peroxyphenylacetic acid) probe, Hammett studies, $H_2{}^{18}O$-exchange experiments, and ESI-mass spectroscopic analysis. Moreover, the nature of solvent significantly influenced partitioning between heterolytic and homolytic O-O bond cleavage of Ni-acylperoxo intermediate (2). The O-O bond of the Ni-acylperoxo intermediate 2 proceeded predominantly via heterolytic cleavage in a protic solvent such as CH_3OH. These results suggested that possibly Ni^{IV}-Oxo species was a common reactive intermediate in protic solvents. The two active oxidants, viz. Ni^{IV}-Oxo (3) and Ni^{III}-Oxo (4), which are responsible for stereospecific olefin epoxidation and radical-type oxidations, respectively, operate in aprotic solvents.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-62**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Photophysical Properties of Iridium(III) Cyclometalates with 1,2-Dihydronaphthyl-Containing C^N Ligands

KUMAR AJAY NGUYEN VAN NGHIA 박재영 이민형*

울산대학교 화학과

Novel Ir(III) cyclometalates, $(dnpz)_2Ir(acac)$ (1c), $(dnpy)_2Ir(acac)$ (2c), and *fac*-$Ir(dnpy)_3$ (2d) (dnpz = 1-(1,2-dihydronaphthalen-4-yl)pyrazole; dnpy = 2-(1,2-dihydronaphthalen-4-yl)pyridine) based on 1,2-dihydronaphthyl-containing C^N Ligands were synthesized and characterized. X-ray diffraction study on 2d revealed facial arrangement of three dnpy ligand around the Ir center. PL spectra of 1c and 2c—2d exhibited yellow to orange emission centered at 539—590 nm, which was red-shifted compared to that (λ_{em} = 508 nm) of *fac*-$Ir(ppy)_3$ (3). While tris-complex 2d showed high quantum efficiency (Φ = 0.57), heteroleptic complexes 1c and 2c were poorly emissive in toluene (Φ = 0.008 and 0.11). In contrast, PLQYs of the film samples of 1c and 2c were much increased (Φ = 0.05 and 0.21). Cyclic voltammetry measurements indicated that the 1,2-dihydronaphthy moiety increased metal-centered HOMO level, while it stabilized LUMO level due to conjugation with *N*-heterocyclic fragments. Details of synthesis, characterization, and photophysical properties of complexes will be discussed.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-63**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A New Zn-MOF Catalyst Containing 3,3'-(Pyrazine-2,5-diyl)dibenzoic Acid Ligand and DABCO

김현철 김성진[1] 김영미[2] 허성[*]

한국외국어대학교 화학과 [1]이화여자대학교 화학과 [2]이화여자대학교 화학-나노과학과

We have constructed a new heterogeneous Zn-MOF catalyst with Lewis basic sites. The Zn-MOF containing ditopic 3,3'-(Pyrazine-2,5-diyl)dibenzoic acid (3,3'-PDBA) linker and 1,4-diazabicyclo[2.2.2]octane (DABCO) has N-atom rich environmental 1D channels. Uncoordinated N atoms of both DABCO and 3,3'-PDBA may show synergistic effect in Lewis basic catalytic activities for nitroaldol reaction, cyanosilylation and Knoevenagel condensation of p-nitrobenzaldehyde. The Zn-MOF based heterogeneous catalytic system for the cyanosilylation revealed recyclability without losing its activity.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-64**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Oxidative addition of dihaloaryl derivatives toward Pd(0) compounds to give mono or dinuclear Pd(II) complexes containing aryl derivatives

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강릉원주대학교 화학과 [1]강릉원주대학교 생명화학공학과 [2]성균관대학교 화학과

Mono or dinuclear Pd(II) halogen complexes containing various aryl derivatives were prepared from oxidative addition of dihaloaryl derivatives to a Pd(0) complex. For example, oxidative additions of various dihaloaryl derivatives to [Pd(CH_2=CHPh)(PR_3)$_2$], which could be generated in situ from trans-[PdEt$_2$(PR_3)$_2$] (PR_3 = PMe_3, PEt_3) and styrene, gave the mono or dinuclear Pd(II) complexes containing haloaryl derivatives depending on the chemical equivalents. Isolated complexes were characterized from spectroscopic and analytical methods. Experimental details will be presented.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-65**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, structure and chemical properties of *cis*-(R or S)-(BINAP)bis(azido)palladium(II): *cis*-[Pd(R or S)-BINAP)(N_3)$_2$]

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강릉원주대학교 화학과 [1]성균관대학교 화학과

New Pd(II) azido complexes containing (R or S)-BINAP (2,2’-bis(diphenylphosphino)-1,1’-binaphthyl) were prepared from reactions of the corsponding (BINAP)$PdCl_2$ with excess NaN_3. Full characterization of the obtained products by IR, NMR, and elemental analyses including X-ray crystallography were carried out. Also, we examined chemical treatments of *cis*-[Pd(R-BINAP)(N_3)$_2$] with organic isothiocyanates (R-N=C=S) and isocyanides(CN-R). Experimental detail will be presented.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-66**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Luminesence Vapochromism by Fast Guest Exchange of Copper(I) Coordination Polymers

박현진 권은진 임한수 김태호* 김진은*

경상대학교 화학과

Six Cu(I) Coordination Polymers (CPs) $[Cu_2I_2L_2]_n$ (**1**), $\{[Cu_2I_2L_2]\bullet MeCN\}_n$ (**2**), $[Cu_4I_4L_2]_n$ (**3**), $\{[Cu_4I_4L_2]\bullet CH_2Cl_2\}_n$ (**4**), $\{[Cu_4I_4L_2]\bullet CHCl_3\}_n$ (**5**) and $\{[Cu_4I_4L_2]\bullet C_6H_6\}_n$ (**6**) have been synthesized by self-assembly reaction of CuI and a flexible ligand with mixed N/S donors, 4-(2-(cyclohexylthio)ethoxy)pyridine(**L**). CPs **1-6** were crystalized in space group Triclinic P-1. Single-crystal X-ray differaction analyses showed that 1D CPs **1–2** and **3-6** are supramolecular isomers based on rhomboid Cu_2I_2 and cubane Cu_4I_4 clusters, respectively. CPs **1** and **2** show emission maxima 419 nm and 432 nm, respectively. CPs **3-6** show emission maxima 535 nm, 539 nm, 542 nm and 546 nm, respectively. Crystal-to-crystal transformations between CPs **1-6** were reversible under appropriate solvent conditions (acetonitrile or dichloromethane or chloroform or benzene) or heat. Also, crystal transformations between CPs **1** and **3** occur through the addition of **L** or CuI. Moreover, CPs **3-6** exhibited reversible guest exchange and crystal transformation by exposure to gaseous volatile organic compounds and heat.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-67**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Luminescence Mechanochromism of a Cu(I) Coordination Polymer without Phase Transition

권은진 박현진 임한수 김진은* 김태호*

경상대학교 화학과

A Cu(I) coordination polymer, $[Cu_2I_2\mathbf{L}_2]_n$ (CP **1**), was prepared by the reaction between CuI and 3-(2-(benzylthio)ethoxy)pyridine (**L**). CP **1** shows luminescence mechanochromism with a color change from greenish-blue to yellow upon the application of pressure. No new peak was observed in Powder X-ray diffraction (PXRD) patterns, indicating non-phase-transition process. The *d*-spacing value of the (111) lattice plane was 7.96, 7.99, and 8.09 Å at 0, 0.05, and 0.4 GPa, respectively. The Raman peaks corresponding to Cu-I, N-Cu, I-I, and Cu-Cu vibration shift from 128.2, 174.3, 208.0, and 253.4 cm^{-1} to 123.8, 169.8, 206.5, and 252.3 cm^{-1}, respectively. PXRD and Raman studies reveal that the changes in the bond lengths in crystalline CP **1** are the main cause of luminescence mechanochromism. After the addition of several drops of acetonitrile to the ground and compressed samples, the original greenish-blue emissive and crystalline states are restored. Therefore, the luminescence color conversion processes are fully reversible

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-68**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Photophysical and Structural Propreties of Copper Iodide Polymorphic Complexes

임한수 권은진 박현진 김태호* 김진은*

경상대학교 화학과

Two copper iodide complexes [$Cu_4I_4L_4$](**1**) and [$Cu_4I_4L_4$](**2**) of benzyl(methyl)sulfane(**L**) have been successfully synthesized and structurally characterized by single crystal X-ray diffraction. Complexes **1** and **2** were crystallized in the space group orthorhombic $P2_12_12_1$ and tetragonal I-4, respectively. Complexes **1** and **2** show a discrete complex based on cubane Cu_4I_4 units. Complexes **1** and **2** are polymorphic complexes. They have different structures with the same formula. Complexes **1** and **2** have different packing structure and intermolecular interactions. Luminescence spectra of the complexes **1** and **2** exhibit emission peaks at 530 nm and 546 nm at room temperature, respectively.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-69**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Identification of multi-step mechanism of cysteine-induced sulfidation by plasmonic monitoring

박영찬 오현철 송현준*

KAIST 화학과

Recent advances in dark-field microscopic imaging analysis technique using plasmonic nanoparticles have enabled the monitoring of chemical reactions in a real-time at a single-particle level. Here, we observed interaction between cysteine and silver nanoparticle from adsorption process to the further sulfidation reaction using dark-field microscopy with flow-cell setup for in situ monitoring. We revealed that the overall reaction of cysteine-induced sulfidation is limited by three different mechanisms: (1) diffusion of cysteine from bulk to silver surface, (2) cysteine decomposition (or sulfidation), and (3) inter-diffusion between silver and silver sulfide. Moreover, kinetic parameters such as activation energy and diffusion constant were calculated. Consequently, these findings provide deeper understanding of the reaction mechanism leading to a new synthetic strategy in bulk system. Our result prove that dark-field microscopic imaging analysis technique can analyze not only simple single reaction but also mixed multi-step mechanism. We expect this method could be used to study more complex reactions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-70**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Thermal electric properties of solution processed antimony-doped tin oxide thin film

김다인 김현성*

부경대학교 화학과

Antimony-doped tin oxide (ATO) nanoparticles with various doping amount of antimony were prepared by solvothermal synthesis. And ATO thin film was fabricated on the glass substrate by spin coating ATO nanoparticles solution. Importantly, these obtained thin films can be annealed at temperature (T_a) from 300 ºC to 500 ºC and afford devices with excellent thermal electrical characteristics. Optimized doping amount of antimony of 1 mol % and T_a= 300 ºC afford ATO thin film exhibiting Seebeck coefficient(S). Remarkably, ATO thin film processed at 500 ºC still exhibit power factor ($S^2 \bullet \sigma$)> 64.4µW/m·K^2, which is encouraging for solution-processing with inexpensive and easy procedures.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-71**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Self-Assembled Ruthenium Heterometallic Supramolecular Architectures Based on Tetratopic N-Donor Metalloligands

류지연 위은혜 이준승*

전남대학교 화학과

For coordination-driven self-assembly, unique tetratopic N-donor metalloligands containing Co or Fe metals were synthesized and used in the construction of unexpected heterometallic supramolecular architectures. These cages were prepared from 2 equiv. of tetrapyridyl star connector as electron donors and 4 equiv. of di-ruthenium acceptors, isolated in good yield and fully characterized by infrared spectroscopy, multinuclear ^{1}H-NMR spectroscopy, high-resolution electrospray ionization mass analysis. Furthermore, solid state structures of these complexes were determined by X-ray crystallography. It reveals that selective [2 + 4] or [3 + 6] self-assembly was achieved by the assembly. Additionally, interesting triple-decker type bimetallic supramolecule was observed.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-72**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Methane to methanol conversion over faujasite zeolites encapsulated copper-phthalocyanine

유혜진 김현성*

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 copper-phthalocyanine in the supercages of faujasite zeolites via “*ship-in-a-bottle*” procedure. Prepared copper-phthalocyanine zeolites composite was shown to be higher oxidative catalytic activity than the authentic homogeneous catalysts under reaction conditions. Herein, methane was partial oxidized to methanol through copper-phthalocyanine zeolite using nitrous oxide as oxidant. We evaluated the effect of zeolite size and Si/Al ratio of its framework on the catalytic performance.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-73**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Di-Ruthenium Acceptor having additional binding sites and their Self-assembly

위은혜 류지연 이준승*

전남대학교 화학과

In the supramolecular chemistry, there have been considerable efforts to find the complicated huge supramolecules which are easy to control. To date, coordination driven self-assembly has used electron donors and acceptors for the construction of supramolecules. To achieve more complicated system, we designed di-ruthenium electron acceptor unit possessing electron donating pyridine units. These complexes could have a dual role as a donor and a accepter to promote additional complexation.Three different kinds of ligands and corresponding metalloligands were synthesized and characterized fully including X-ray crystallography. Simple self-assembly to rectangles and further complexations with additional metal precursor to construct complicated huge supramolecules will be presented.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-74**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and characterization of Cu(II) and Zn(II) complexes bearing (+)-Camphor derivative of (E)-1-(2-Pyridyl)ethylamine

조주현 정종화*

경북대학교 화학과

The discovery and development of novel chiral ligands are of significant importance in asymmetric catalysis. So we were synthesized α-methyl-N-[(1R, 4R)-1,7,7-trimethylbicyclo-[2.2.1]hept-2-ylidene]-(E)-1-(2-pyridyl)ethylamine (PIC) ligand and characterized. This ligand has led to C1-symmetric ligand with two differentiated N (sp2) atoms and provide highly sterically differentiated surroundings for both equatorial coordination sites of the metal ion [Cu(II), Zn(II)]. The X-ray crystal structure of Cu(II) and Zn(II) complex containing PIC was determined. (1R,4R)(S) and (1R,4R)(R)-coordination Cu(II) and Zn(II) complexes were cocrystallized. The geometry around the Cu(II) centre for (PIC) CuCl2 was distorted square-planar and Zn(II) centre for (PIC)ZnCl2 was distorted tetrahedral.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-75**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Characterization of Zn(II) and Cu(II) Complexes Bearing Ethanediamine-diethyl-[(1R)-1-phenylethyl] Derivative

강미성 정종화*

경북대학교 화학과

New Zinc(II) and Copper(II) complexes based on bidentate ligand [1,2-Ethanediamine, N1,N1-diethyl-N2-[(1R)-1-phenylethyl]](EDADEPE) have been synthesized in high yield and purity. Ligand was characterized by 1H-NMR and 13C-NMR and the crystal structures of the Zn(II) and Cu(II) complexes were determined by X-ray crystallography. The X-ray structures showed that the stereogenic nitrogen and carbon atoms were RC and SN in (EDADEPE)ZnCl2. The geometry around the Zn(II) centre for (EDADEPE)ZnCl2 was tetrahedron which was slightly distorted. On the other hand, Cu(II) complex has a cocrystallized complex which the X-ray showed (RC, RN) and (RC, SN)-coordination complexes. Both of their geometry around the Cu(II) centre for (EDADEPE)CuCl2 were distorted square-planar.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-76**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fully Ordered $L1_0$-FePt Nanoparticles with Controlled Pt-Shell Thicknesses for Electrochemical Methanol Oxidation Reaction

홍용훈 서원석*

서강대학교 화학과

We present a simple one-step approach to the synthesis of ~4 nm uniform and fully $L1_0$-ordered face-centred tetragonal (fct) FePt nanoparticles (NPs) embedded in ~60 nm MCM-41 (fct-FePt NPs@MCM-41). We controlled the Pt-shell thickness of the fct-FePt NPs by treating fct-FePt NPs@MCM-41 with acetic acid (HOAc) or hydrochloric acid (HCl) under sonication, thereby etching the surface Fe atoms of the NPs. The fct-FePt NPs deposited onto the carbon support (fct-FePt NP/C) were prepared by mixing the fct-FePt NPs@MCM-41 with carbon and subsequently removing the MCM-41 using NaOH. Additionally, we developed a facile method to synthesize acid-treated fct-FePt NP/C by using a HF solution for simultaneous surface-Fe etching and MCM-41 removal. We have studied the effects of both surface-Fe etching and Pt-shell thickness on the electrocatalytic properties of fct-FePt NPs for the methanol oxidation reaction (MOR). Compared with the non-treated fct-FePt NP/C catalyst, the HOAc-treated and HCl-treated catalysts exhibit up to 34% larger electrochemically active surface areas (ECASAs); in addition, the HCl-treated fct-FePt NP (with ~1.0 nm Pt shell)/C catalyst exhibits the highest specific activity. The HF-treated fct-FePt NP/C exhibits an ECASA almost 2 times larger than those of the other acid-treated fct-FePt NP/C catalysts and shows the highest mass activity (1,435 mA $mgPt^{-1}$, 2.3 times higher than that of the commercial Pt/C catalyst) and stability among the catalysts tested. Our findings demonstrate that surface-Fe etching for the generation of the Pt shell on fct-FePt NPs and the Pt-shell thickness can be factors for optimizing electrocatalysis of the MOR.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-77**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Superamolecular Arrays of Metallacyclodimeric Zn(II) Complexes: Solvent Recognition

이정준 이다슬 정옥상*

부산대학교 화학과

Self-assembly of ZnX_2 (X = Cl, Br, and I) with bidentate Ligand (L) as a hemi-circular bidentate ligand containing chromophore moiety yields a systematic 46-membered metallacyclodimeric unit, $[ZnX_2(L)]_2$. These basic skeletons constitute, via interdigitated $\pi\cdots\pi$ interactions in a staggered fashion, a unique ensemble forming both channels and cages. Specifically, the ensemble with channel and cage significantly stabilizes the solvate molecules. The unprecedented supramolecular structures adsorb/desorb small solvent molecules.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-78**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Constructions and Catalytic Properties of Enantiomeric Two-fold 3D Zinc(II) Coordination Networks

이해리 정옥상*

부산대학교 화학과

Self-assembly of $Zn(ClO_4)_2$ with 1,1,2,2-tetramethyl-1,2-di(pyridin-3-yl)disilane (L) as a bidentate *N*-donor gives rise to 3D coordination networks, $[Zn(\mu\text{-}OH)(L)]_3(ClO_4)_3\cdot 5H_2O$, of unique, 10^3-a *srs* net topology. An important feature is that two enantiomeric 3D frameworks, 4^1- and 4^3-$[Zn(\mu\text{-}OH)(L)]_3(ClO_4)_3\cdot 5H_2O$, are interpenetrated to form a racemic two-fold 3D network with cages occupied by two water molecules. Another structural characteristic is a C_3-symmetric planar $Zn_3(\mu\text{-}OH)_3$ 6-membered ring with tetrahedral Zn(II) ions. The steric hindrance of substrates and trace water effects on transesterification catalysis using the network has been scrutinized. For the reaction system, solvate water molecules within the cages of the interpenetrated 3D frameworks do not decrease the transesterification activity, whereas the trace water molecules in the substrate alcohols act as obvious obstacles to the reaction. The significantly different effects between the water molecules inside and outside of the oval-shaped cage represent an important conceptual advance in the development of such a catalytic system. More systematic studies, for example on the synthesis of related ligands, are in progress. Further investigation of this series of coordination frameworks, including a new topology based on the *N*-donor tridentate ligand, also is underway.

Reference

[1] Choi, E.; Ryu, M.; Lee, H.; Jung, O.-S. *Dalton Trans.* **2017**, *submitted*

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-79**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Solvent-Template Effects on Coordination Polymerization of Cadmium(II) Complexes

류민주 정옥상*

부산대학교 화학과

Self-assembly of cadmium(II) chloride with new bidentate ligand (L) in different solvent system has been achieved. The self-assembly reactions show significant solvent template effects. Each reaction gives rise to form the composition of Cd(II) : L (1 : 2).

The reaction in acetonitrile yields 1D loop chain of $[CdCl_2L_2]\cdot 2CH_3CN$.

The reaction in MeOH yields 1D loop chain of $[CdCl_2L_2]\cdot 4CH_3OH$.

The reaction in EtOH yields interpenetrated 2D sheet of $[CdCl_2L_2]$.Constructions of each structure are determined by solvents rather than synthetic methodologies. For some structures, exchange of the solvate molecules in the crystalline solids is carried out, and the 1D skeletal structure discriminates dioxane and CH_2Cl_2 molecules.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-80**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Suprachannels via a Molecular Array of 2D Networks consisting of Ag(I) and Tridentate *N*-donor Ligands

최다예 황서영 정옥상*

부산대학교 화학과

Self-assembly of Ag(I)X (X = PF_6^-, CF_3SO_3) with tridentate ligand in a mixture solvent system gives rise to crystals of $[Ag_2L_2(THF)_2](PF_6)_2\cdot THF$ and $[Ag_3(OTf)_3L_3]\cdot 3THF\cdot H_2O$, respectively. Their structures are a 2D network consisting of 54-membered metallacyclic unit. Exchanges of the solvate molecules in both the crystalline solids and desolvated solids are carried out, and the 2D skeletal structure discriminates dioxane and CH_2Cl_2 molecules. The 2D networks are arranged in an eclipsed mode in aqueous solution, thus forming suprachannels of $[Ag_3L_2(H_2O)_2](X)_3$, whereas they are arranged in a staggered abab··· mode in non-aqueous solution, thus forming semi-suprachannels of $[Ag_3(NO_3)_2L_2](NO_3)$. In the present study, significant differences in solvent recognition and anion between $[Ag_3L_2(H_2O)_2](NO_3)_3$ and $[Ag_3(NO_3)_2L_2](NO_3)$ were found.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-81**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Photoluminescence Recognition of Diiodomethane using Zn_3L_2 Complex

이상석 정옥상*

부산대학교 화학과

Discrete M_3L_2 structure, $[Zn_3(\mu\text{-}OH)_3L_2](ClO_4)_3\cdot 4CH_3CN\cdot 2H_2O$ was successfully synthesized through self-assembly of $Zn(ClO_4)_2$ with 1,3,5-tris(dimethyl(pyridin-3-yl)silyl)benzene (L). Its blue photoluminescence is significantly quenched by only CH_2I_2 among various small molecules such as CH_2Cl_2, CH_2Br_2, $CHCl_3$, 1,2-dichloroethane, EtOH, MeOH, CH_3CN, benzene, toluene, and phenol.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-82**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Diiridium (III) complexes as luminescent probes and sensors for G-quadruplex DNA and endoplasmic reticulum imaging

김진홍* **TIKUM FLORENCE ANJONG**[1] 임윤진[2]

이화여자대학교 화학·나노과학과 [1]이화여자대학교 화학나노과학과 무기화학전공 [2]이화여자대학교 화학나노과학과

G-quadruplex is a four stranded structure, derived from a guanine (G) rich DNA sequence. Though G-rich sequences have been demonstrated to form g-quadruplex structure invitro, the existence of g-quadruplex structure invivo is still controversial. Thus detecting g-quadruplex structure has great significance for cell proliferation, cancer research and drug development. Also, imaging of small organelles in the cell such as ER is very important, in understanding the structure and function of these organelles. Herein, two new dinuclear iridium (Ir) complexes bridged by a conjugate aromatic tppz ligand, were prepared. The DNA binding properties of both complexes where studied using single, double stranded and g-quadruplex DNA. Interestingly, the Ir complex demonstrated selectivity for g-quadruplex DNA over other control DNA which was observed by an enhancement in the phosphorescent spectra of 1. Inorder to understand their possible interaction with lipid-rich organelles in live cells, the phosphorescent properties of both complexes were studied using liposomes which showed an increased in phosphorescent intensity upon the addition of liposomes with complex showing a greater enhancement. The complex could be used as probes in live cells. Complexes were intensely stained in HeLa cervical cancer cells. Excitation with a l = 488 nm laser showed red emission localized in the cytosol of cells. Cellular studies showed that 1 and 2 were located inside HeLa cells, but neither complex passed through the nuclear membrane. However, complexes possessed superior photostability, indicating their role as good luminescent agents for imaging and tracking the endoplasmic reticulum in live cells. Overall, the complex exhibited better selectivity for G-quadruplexes, liposomes, and ER staining.

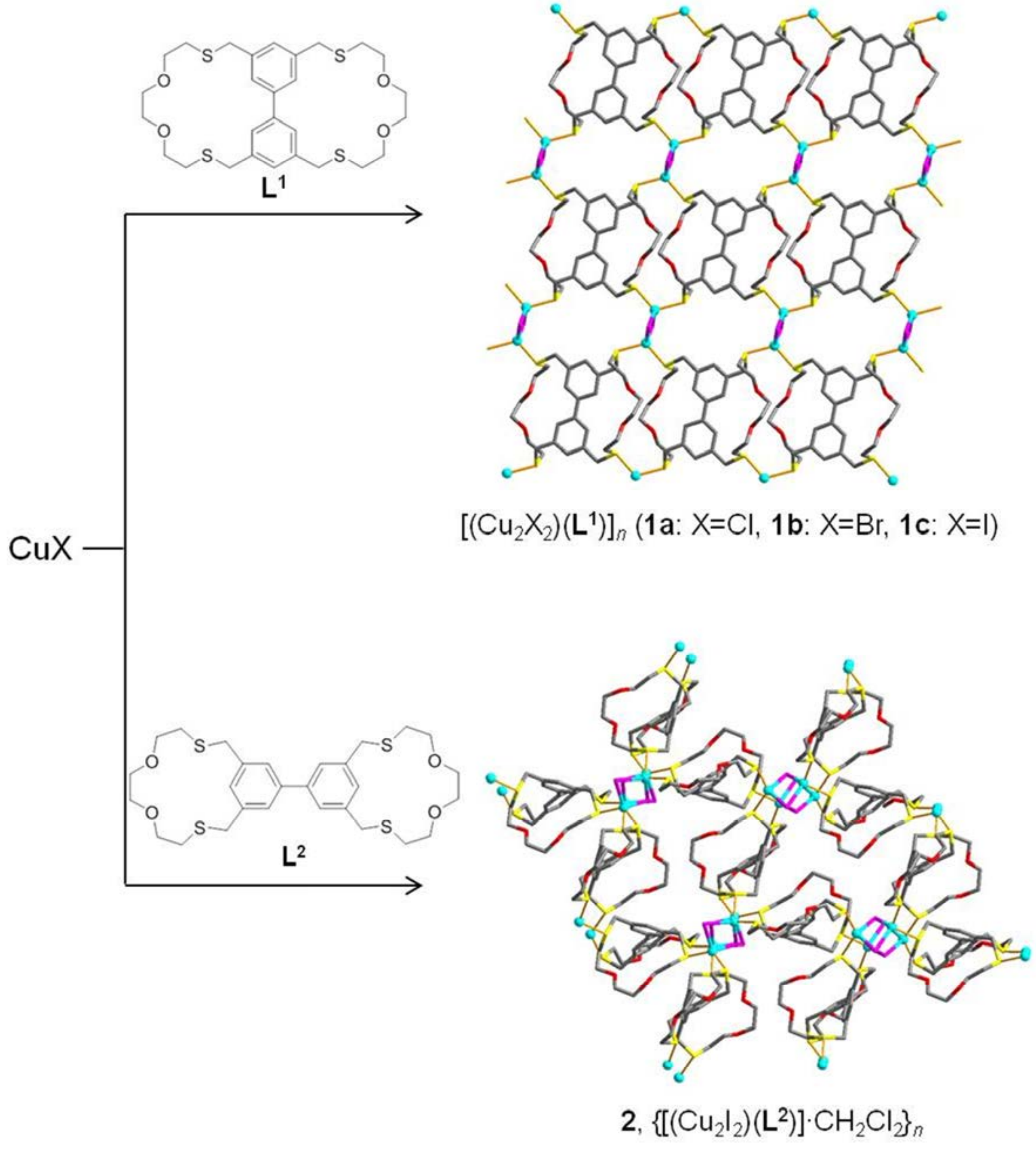
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-83**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of Bis-Thiamacrocycle Isomers Incorporating Rotating Axis and Their Soft Metal Complexes

김슬기 이심성*

경상대학교 화학과

Coordination behaviors of the bis-thiamacrocycle isomers incorporating a biphenyl subunit exhibiting different rotating barriers are reported. A mixture of region-isomers $\mathbf{L^1}$ and $\mathbf{L^2}$ was synthesized via the corresponding one-pot coupling reactions of 3,3',5,5'-tetrakis(bromomethyl)biphenyl with 3,6-dioxa-1,8-octanedithiol and separated using a column chromatography. $\mathbf{L^1}$ reacts with copper(I) halides to afford an isostructural 2D polymeric products, $[(Cu_2X_2)(\mathbf{L^1})]_n$ (**1a**: X=Cl, **1b**: X=Br, **1c**: X=I), in which the macrocycles are linked by square-type Cu_2I_2 clusters via an exocyclic coordination mode. Meanwhile, reaction of $\mathbf{L^2}$ with CuI afforded a 2D polymeric network, $\{[(Cu_2I_2)(\mathbf{L^2})]\cdot CH_2Cl_2\}_n$ (**2**), doubly linked by the Cu_2I_2 clusters with different connectivity pattern. The topological analysis of **1** and **2** shows **sql** and **4,4L1** topologies, respectively.


L1
CuX
L2
[(Cu2X2)(L1)]n (1a: X=Cl, 1b: X=Br, 1c: X=I)
2, {[(Cu2I2)(L2)]·CH2Cl2}n

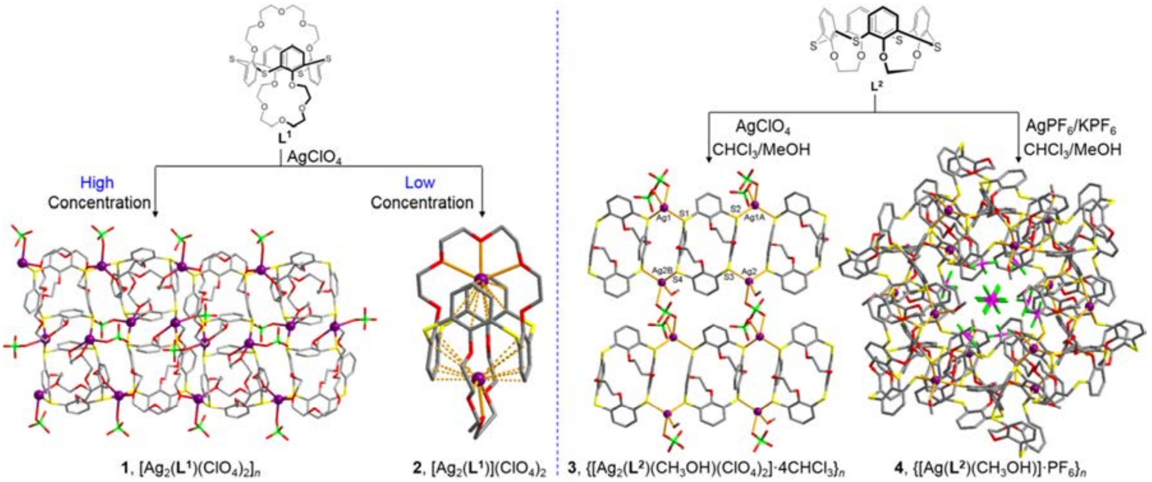
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-84**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Silver(I) Complexes of Thiacalix[4]-bis-crown and Its Unprecedented Basket-Type Derivative

주희영 이심성*

경상대학교 화학과

Thiacalix[4]-bis-crown ($\mathbf{L^1}$) and its basket-type derivative ($\mathbf{L^2}$) were employed and their silver(I) complexes with different topologies are reported. Reaction of $\mathbf{L^1}$ (~10 mM) with three equivalents of $AgClO_4$ in a mixture of chloroform-methanol afforded an exo-coordinated one dimensional coordination polymer $[Ag_2(\mathbf{L^1})(ClO_4)_2]_n$ (**1**). When the above synthetic procedure was repeated in a lower concentration of $\mathbf{L^1}$ (~1 mM), a discrete endocyclic disilver(I) complex $[Ag_2(\mathbf{L^1})](ClO4)_2$ (**2**) was isolated. On the other hand, tetra-toylated thiacalix[4]arene was found to undergo unprecedented intramolecular cyclization to yield the basket-type derivative $\mathbf{L^2}$. The mechanism of the basket compound $\mathbf{L^2}$ via the two stage detosyl and interconversion of the aromatic units is proposed. Using $\mathbf{L^2}$, two silver(I) complexes with different anions (**3**: ClO_4^- and **4**: PF_6^-) have been isolated. The ClO_4^- complex **3**, $\{[Ag_2(\mathbf{L^2})(CH_3OH)(ClO_4)_2]\cdot 4CHCl_3\}_n$, shows an exo-coordination based 2D infinite structure, in which the anion acts as a linker. The corresponding PF_6^- complex **4**, $\{[Ag(\mathbf{L^2})(CH_3OH)](PF_6)\}_n$, exhibits a multichannel type 3D framework, in which the single channels are further linked by exocyclic silver(I) ions.



1, $[Ag_2(\mathbf{L^1})(ClO_4)_2]_n$ **2**, $[Ag_2(\mathbf{L^1})](ClO_4)_2$ **3**, $\{[Ag_2(\mathbf{L^2})(CH_3OH)(ClO_4)_2]\cdot 4CHCl_3\}_n$ **4**, $\{[Ag(\mathbf{L^2})(CH_3OH)]\cdot PF_6\}_n$

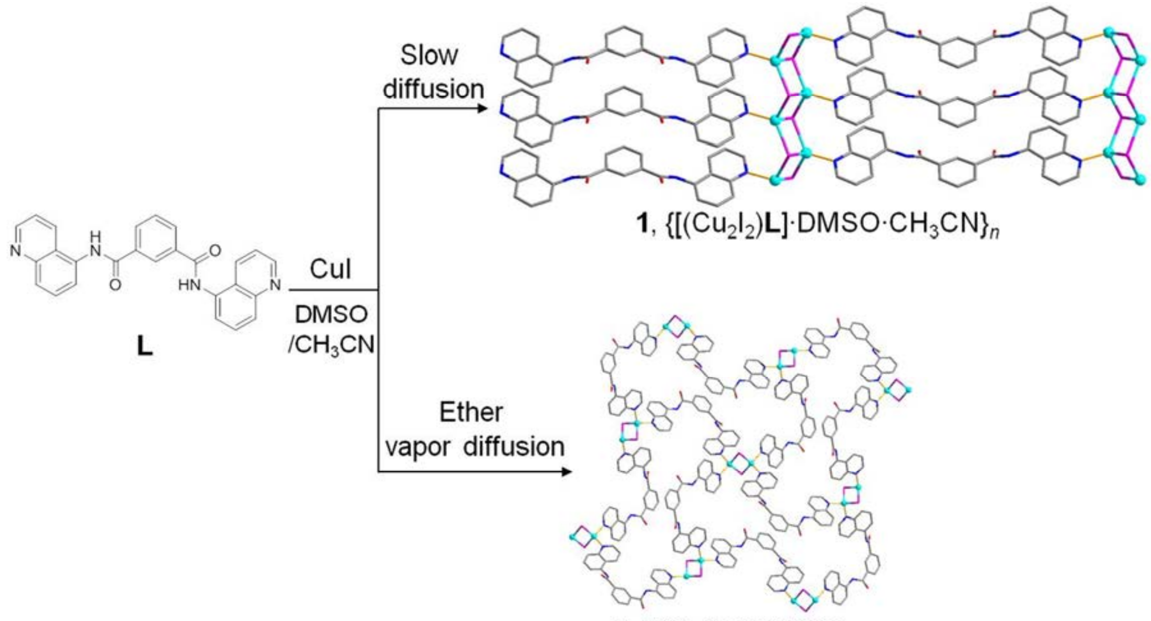
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-85**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Infinite 2D Cu(I) Complexes of Bis(amidoquinoline) Ligand with Different Connectivity Patterns Depending on Reaction Condition

이은지 이심성[1,*]

경상대학교 화학과 [1]경상대학교 화학과

We report the reaction condition-dependent copper(I) iodide complexes **1** and **2**, derived from a bis(amidoquinoline) ligand (**L**)[1]. The complex **1**, $\{[(Cu_2I_2)\mathbf{L}]\bullet DMSO\bullet CH_3CN\}_n$, isolated from the slow diffusion method shows a 2D network with an infinite stair step shaped Cu_nI_n cluster backbone. However, in ether vapor diffusion method, we isolated the complex **2**, $\{[(CuI)\mathbf{L}]\bullet DMSO\}_n$, which shows an infinite 2D network linked by rhomboid-type Cu_2I_2 clusters. Interestingly, the complex **2** was also obtained under the mechanochemical condition in the presence of three drops of CH_3CN and one drop of DMSO. Furthermore, the complexes **1** and **2** exhibit yellow (λ_{em} = 550 nm) and orange (λ_{em} = 590 nm) emission, respectively, via MLCT.



1, $\{[(Cu_2I_2)\mathbf{L}]\cdot DMSO\cdot CH_3CN\}_n$

2, $\{[(CuI)\mathbf{L}]\cdot DMSO\}_n$

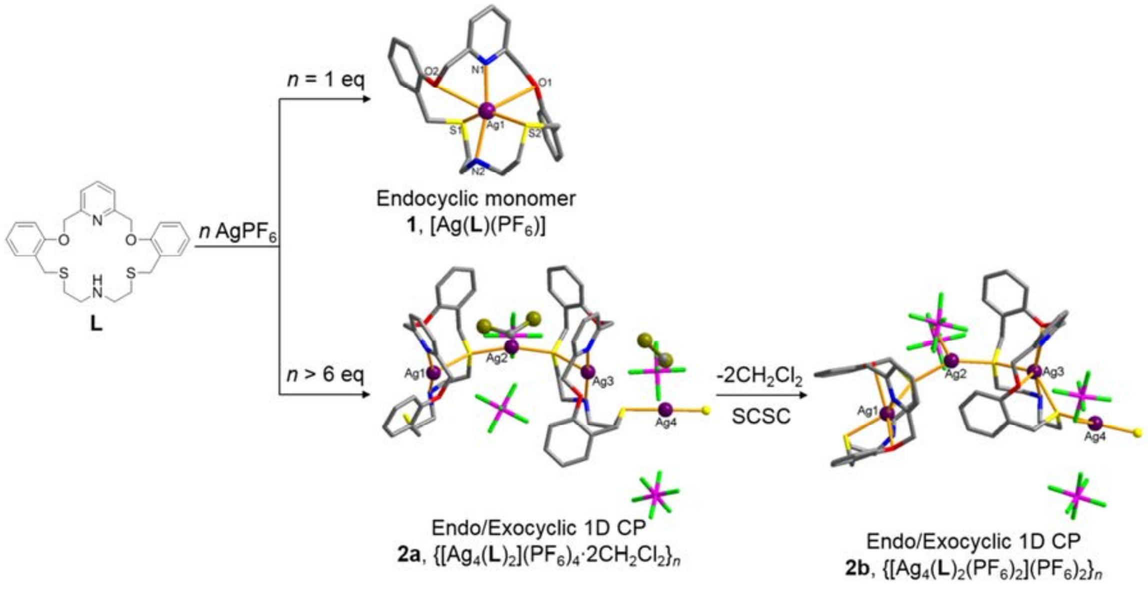
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-86**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Mole-Ratio Dependent Endo/Exocyclic Infinite Silver(I) Complexes with an $N_2O_2S_2$-Macrocycle

서수진 이심성* 이은지

경상대학교 화학과

An $N_2O_2S_2$-macrocycle (**L**)[1,2] incorporating one pyridine and two benzo subunit was employed and their silver(I) and copper(I) complexes are reported. Reaction of **L** with $AgPF_6$ afforded a typical endocyclic complex [Ag(**L**)(PF_6)] (**1**). In the mole-ratio variation experiments, the use of six equivalents or above amount of $AgPF_6$ gave an endo/exocyclic 1D coordination polymer $\{[Ag_4(\mathbf{L})_2](PF_6)_4{\cdot}2CH_2Cl_2\}_n$ (**2a**), in which the endocyclic complex units are linked by the exocyclic silver(I) ions to form an (**L**-Ag)-Ag-(**L**-Ag)-Ag pattern. In addition, when single crystals of **2a** was undisturbed in air, the lattice solvent molecules were removed to form $\{[Ag_4(\mathbf{L})_2(PF_6)_2](PF_6)_2\}_n$ (**2b**) accompanying the change of the coordination environments involving the anions in a single-crystal to single-crystal (SCSC) manner. Meanwhile, reactions of **L** with CuI in the presence of CF_3COOH gave an emissive coordination polymer $\{[Cu_4I_4(\mathbf{L})_2]{\cdot}2CF_3COOH\}_n$ (**3**) with a double-stranded 1D chain structure linked by cubane-type Cu_4I_4 clusters.



L
n AgPF$_6$
n = 1 eq
O2
N1
O1
S1
Ag1
S2
N2
Endocyclic monomer
1, [Ag(L)(PF$_6$)]
n > 6 eq
Ag1
Ag2
Ag3
Ag4
Endo/Exocyclic 1D CP
2a, {[Ag$_4$(L)$_2$](PF$_6$)$_4$·2CH$_2$Cl$_2$}$_n$
-2CH$_2$Cl$_2$
SCSC
Ag1
Ag2
Ag3
Ag4
Endo/Exocyclic 1D CP
2b, {[Ag$_4$(L)$_2$(PF$_6$)$_2$](PF$_6$)$_2$}$_n$

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

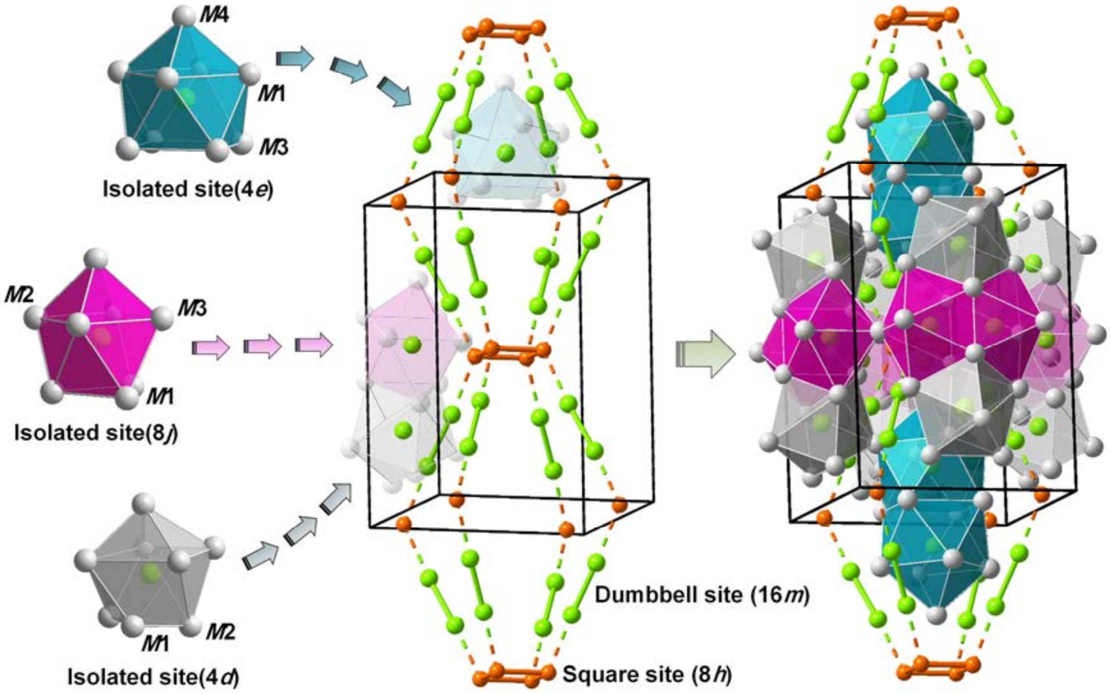
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-87**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Effect of Multi Doping on the Thermoelectric Property of the $Ca_{11-x}Yb_xSb_{10-y}Tt_y$ (Tt = Si, Ge; $1.29 \le x \le 9.65$; $y = 0.25, 0.48$) System

최웅진 이준수 유태수*

충북대학교 화학과

Thermoelectric (TE) materials can be used to convert the wasted heat from many different heat sources into electricity. In recent years, a series of binary and ternary pnictogen containing the small amounts of triels- or tetrels-doping, which include the $A_{11}Pn_{10-x}T_x$ (A = Rb, Cs, Sr, Ba, Eu, Yb; Pn = Sb, Bi; and T = Si, Ge, Sn) systems has also been studied for its thermoelectric applications. In particular, according to the previous article about $A_{11}Sb_{10}$ (A = Ca, Yb) system reported by Prof. Kauzlarich and Prof. Snyder, if a solid-solution system of $Ca_{11-x}Yb_xSb_{10}$ were successfully prepared, then the electronic property could be finely tuned between a metal and a semiconductor as in the $Ca_{1-x}Yb_xZn_2Sb_2$ solid-solution. Therefore, we attempted to make this solid-solution system by introducing the mixed-cations of Ca2+ and Yb2+. In addition, we also allow the system to have the anionic doping as well. Thus, Ge and Sn atoms were introduced to replace some of Sn in the system. Therefore, in this research, we discuss our systematic experimental and theoretical investigations of the effect of multi doping using both of cationic and anionic elements on the quaternary tetrel compounds the $Ca_{11-x}Yb_xSb_{10-y}Tt_y$ (Tt = Si, Ge; $1.29 \le x \le 9.65$; y = 0.25, 0.48) System. These compounds have been synthesized by using either Sn metal-flux or arc-melting and characterized by both powder and single crystal X-ray diffractions. As a result, we expect to see the influence of cationic and anionic doping on the electronic properties as well as thermoelectric properties, the site-preference of cations and anions based on the QVAL values, and the rationale of some historically large ADP values on two particular atomic sites. In addition, we also discuss the results of SEM and EDS, and TGA analyses.


M4
M1
M3
Isolated site(4e)
M2
M3
M1
Isolated site(8j)
M1
M2
Isolated site(4d)
Dumbbell site (16m)
Square site (8h)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-88**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Cobalt(II) and Zinc(II) Complexes Containing *N*'-substituted *N*,*N*',*N*-bis((1H-pyrazol-1-yl)methyl)amine Derivatives: Synthesis, characterization and application towards methyl methacrylate polymerization

신수진 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

We have synthesized new series of Co(II) and Zn(II) complexes with ligands L_n ($L_n = L_A – L_C$) where L_A = *N*,*N*-bis((1H-pyrazol-1-yl)methyl)benzenamine), L_B = *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-3,5-dimethylbenzenamine), L_C = *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2,6-diisopropylbenzenamine). All complexes were characterized by IR, ^{1}H-NMR, ^{13}C-NMR, elemental analyzer, and X-ray single crystal diffraction. Molecular structures of Co(II) and Zn(II) both complexes showed distorted tetrahedral geometry around the corresponding metal center. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were also investigated at 60 °C.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-89**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Structural Characterization of 6-Coordinate Cd(II) Complexes Containing 4-methoxy-*N*-((pyridin-2-yl)methylene)benzenamine Derivatives

박수현 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

We have synthesized and characterized a series of new Cd(II) complexes, namely [L_nCdBr_2] with ligands [L_n] ($L_n = L_A – L_C$), where L_A = 4-methoxy-*N*-((pyridin-2-yl)methylene)benzenamine, L_B = 4-methoxy-*N*-((pyridin-2-yl)methyl)benzenamine, L_C = 4-methoxy-*N*-methyl-*N*-((pyridin-2-yl)methyl)benzenamine. Molecular structure of [$(L_B)_2CdBr_2$] was 6-coordinate octahedral geometry around cadmium metal center. The catalytic properties of Cd(II) complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were investigated at 60 ^{o}C.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-90**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Structural characterization of Cobalt (II) Complexes Containing *N,N*-Bis((1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amines

서재영 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New series of Co(II) complexes, $[L_nCoX]Y$ ($L_n = L_A, L_B, L_C, L_D, L_E, L_F$; X = Cl, NO_3; Y = BPh_4, NO_3) were synthesized by the reaction of metal starting materials such as $[CoCl_2]$ and $[Co(NO_3)_2]$ with the corresponding ligands *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amine (L_A) and *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amine (L_B) and *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-N-methylpropane-1,3-diamine (L_C) and *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-N-methylpropane-1,3-diamine (L_D) and *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2-(pyridin-2-yl)ethan-1-amine (L_E) and *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)-2-morpholinoethan-1-amine (L_F), in the presence of $NaBPh_4$, respectively. Molecular structures of Co(II) complexes were 5-coordinate trigonal bipyramidal geometry around cadmium metal center. The catalytic property of Co(II) complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO were investigated at 60 ^{o}C.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-91**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Zinc(II) Complexes Containing *N*'-Substituted *N*,*N*-Bispyrazolyl Ligands: Application to Polymerizations of methyl methacrylate and Lactide

조형우 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

New complexes [L_nZnCl_2] ($L_n = L_A – L_E$) were synthesized by the reaction of [$ZnCl_2$] with *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-2,6-dimethylbenzenamine (L_A), *N*,*N*-bis((1H-pyrazol-1-yl)methyl)-4-bromobenzenamine (L_B), *N*,*N*-bis((1H-pyrazol-1-yl)methyl)benzhydrylamine (L_C), *N*,*N*-bis((1H-pyrazol-1-yl)methyl)cyclohexylmethylamine (L_D), *N*,*N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)cyclohexylmethylamine (L_E), respectively. Zn(II) complexes were characterized by ^{1}H-NMR, ^{13}C-NMR, IR, and elemental analyzer. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) and racemic lactide were investigated. [L_CZnCl_2] showed the highest catalytic activity for the polymerization of methyl methacrylate (MMA) in the presence of modified methylaluminoxane (MMAO) with an activity of 3.95×10^4 g PMMA/molcat•h at 60^{o}C. Methylated Zn(II) complexes were employed and evaluated as an initiator for ROP of *rac*-Lactide. The heterotactic polylacticacid (PLA) with P_r up to 79 % can be obtained in CH_2Cl_2 at -50^{o}C.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-92**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

N-substituted 2-iminomethylquinoline and 2-iminomethylpyridine coordinated Zinc(II) complexes: Synthesis, structural characterization and application to polymerization of methyl methacrylate

허정 이효선[1,*]

경북대학교 화학과 [1]경북대학교 자연과학대학 화학과

We have synthesized and characterized a series of zinc(II) complexes, namely [L_nZnCl_2] with ligands [L_n] (L_n = L_A – L_D), where (L_A, = *N*-(quinolin-2-ylmethylene)cyclopentanamine), (L_B = *N*-(quinolin-2-ylmethylene)cyclohexanamine), (L_C = *N*-(pyridin-2-ylmethylene)-2-furanmethanamine), (L_D = 2,6-diethyl-*N*-(pyridin-2-ylmethylene)aniline). X-ray single crystal diffraction revealed that all Zn(II) complexes have distorted tetrahedral geometry around the zinc metal center. The catalytic activity of these complexes towards the polymerization of methyl methacrylate (MMA) in the presence of MMAO were investigated at 60 ℃. Specifically, [L_BZnCl_2] showed the highest catalytic activity (2.81 g/molZn•h×10^4) for the polymerisation of methyl methacrylate (MMA) among the others.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-93**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Colorimetric detection of Fe3+ and Fe2+ and sequential fluorescent detection of Al3+ and pyrophosphate by an imidazole-based chemosensor in a near-perfect aqueous solution

윤진영 채주병 김 철[1,*]

서울과학기술대학교 정밀화학과 [1]서울과학기술대학교 정밀화학과 친환경소재제품센터

A novel chemosensor was designed and synthesized for various analytes: Fe3+, Fe2+, Al3+ and pyrophosphate. The sensor showed a selective color change from yellow to orange toward both Fe3+ and Fe2+ in a near-perfect aqueous solution, which could be reusable simply through treatment with ethylenediaminetetraacetic acid. The detection limits (0.27 μM and 0.32 μM) for Fe3+ and Fe2+ were much lower than the environmental protection agency guideline (5.37 μM) in drinking water. The sensor could be used to quantify Fe3+ in real water samples. Moreover, this sensor acted as a 'turn-on' and 'turn-off' type fluorescent sensor toward Al3+ and pyrophosphate. The sensing mechanism of the sensor for Al3+ could be explained by chelation-enhanced fluorescence effect, which was supported by theoretical calculations. Through a metal-complex displacement method, the sensor-Al3+ complex selectively responded to pyrophosphate over various anions especially including phosphate-based anions. Interestingly, the sensor could be used to sequentially detect both Al3+ and pyrophosphate in the living cells.

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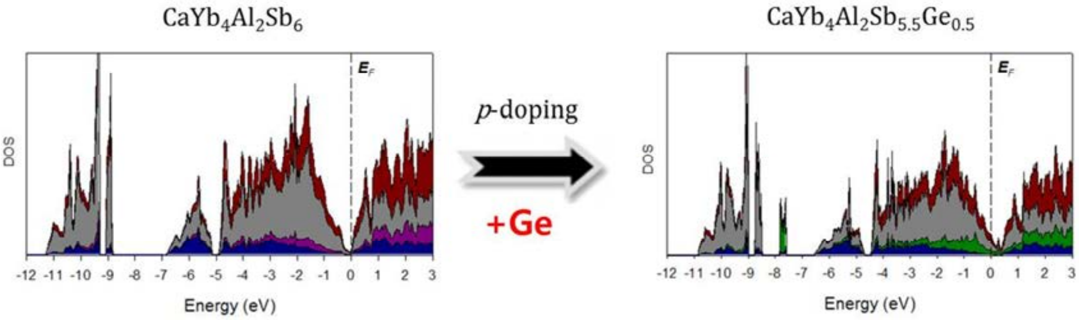
장소: 일산 KINTEX
발표코드: **INOR.P-94**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Two Strategic Approaches to Enhance the Thermoelectric Property of the Zintl Phase $Ca_{5-x}Yb_xAl_2Sb_{6-y}Ge_y$ System

임성지 유태수*

충북대학교 화학과

The solid-solution Zintl compounds with the mixed cations of $Ca^{2+}$and Yb^{2+} in the $Ca_{5-x}Yb_xAl_2Sb_6$ ($1.0 \leq x \leq 5.0$) system have been known to be synthesized by the arc-melting method, and two slightly different crystal structures of the $Ba_5Al_2Bi_6$-type and $Ca_5Ga_2Sb_6$-type phases have been characterized using powder and single-crystal X-ray diffractions. The two phases adopt the orthorhombic space group *Pbam* (Z = 2, *oP26*) with seven independent asymmetric atomic sites in a unit cell. In our earlier investigations, we revealed that the $Ca_5Ga_2Sb_6$-type phase showed a better thermoelectric performance than that of the $Ba_5Al_2Bi_6$-type phase. With this Zintl compound, two strategies to improve ZT value have been attempted. One is the Sb/Ge anion mixing to introduce a hall doping for the $Ca_5Ga_2Sb_6$-type phase, and the other one is an introducing of a phase segregation from a parent $Ca_5Ga_2Sb_6$-type phases into a mixture containing a $Ba_5Al_2Bi_6$-type as well. For the Sb/Ge anion-mixing study, several compounds in the $Ca_4YbAl_2Sb_{6-y}Ge_y$ system containing different ratios of Sb and Ge were synthesized by arc melting. After then, the compounds underwent the phase transition from the $Ba_5Al_2Bi_6$-type to the $Ca_5Ga_2Sb_6$-type structure via annealing process at 700°C for 2 weeks. The resultant compound indeed shows an enhanced ZT value implying the hole doping was partial successful. For a phase-segregation study, as synthesized $Ca_{1.5}Yb_{3.5}Al_2Sb_6$ underwent an annealing process for various durations from one to three days. Once the two title phases were observed in powder X-ray diffraction experiment, a series of thermoelectric property measurements were conducted.


$CaYb_4Al_2Sb_6$
$CaYb_4Al_2Sb_{5.5}Ge_{0.5}$
DOS
E_F
p-doping
+Ge
-12 -11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3
Energy (eV)

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-95**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Microporous and Hollow Organic Polymers with Sulfonic Acids Groups as Antifouling Seed Materials for Polyketone Synthesis

강신영 손성욱*

성균관대학교 화학과

This presentation will show the synthesis of hollow and microporous organic polymers (HMOPs) using zeolitic imidazolate framework (ZIF-8) as a template. Sulfonic groups were incorporated into HMOPs via a post synthetic method. The final material, HMOP-SO_3H is applied as antifouling seeds and efficient catalyst activator for polyketone synthesis. Polyketones are thermoplastic polymers which have been produced in methanol using CO, ethylene, and Pd catalysts. One of the main obstacles for managing continuous synthetic process of polyketone is the reactor fouling that raises synthetic costs and reduces the bulk density of polymers. To solve an antifouling problem, seed materials have been added to the reaction media. The HMOP-SO_3H showed high dispersibility in organic solvent and excellent performance as heterogeneous seed materials in polyketone synthesis. Through screening the synthetic conditions, it was found that a very small amount of HMOP-SO_3H showed successful antifouling performance, compared to the conditions of industrial cases. According to PXRD analysis, the polyketones prepared by HMOP-SO_3H showed α phase more dominantly than β phase, which means that polyketones are crystallize more gradually by seed mediated polymerization.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-96**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, structure determination, characterization and magnetic property of a new lithium manganese selenite

조홍일 옥강민*

중앙대학교 화학과

A new lithium manganese selenite has been synthesized by hydrothermal and solid state reactions using Li_2CO_3, Mn_2O_3, and SeO_2. A hexagonal crystal was used to determine the crystal structure using single crystal X-ray diffraction. The selenite crystallizes in the rhombohedral space group, R-3. The selenite reveals a zero dimensional structure consisting of MnO_6 octahedra, SeO_3 trigonal pyramids, and Li^+ ion. Mn^{3+} cations is are surrounded by six $Se(1)O_3^{2-}$ ions, which forms $Mn(SeO_3)_6$ octahedral structures. Regarding Li-O bond as a covalent bonding, while Li(1) and Li(2) forms LiO_4 tetrahedral environment with oxide ligands, and Li(3) builds LiO_6 trigonal antiprisms. $Li(3)O_6$ is connected with six $Li(2)O_4$ tetrahedra by edge- sharing along the ab-plane. Two $Li(1)O_4$ makes share their edges through O(4) and form a $Li(1)_2O_6$ dimer by edge sharing through O(4) and the dimer are is further bonded to $Li(2)O_4$ via O(2). $Se(2)O(4)_3$ is linked to $Li(1)_2O_6$ and $Li(2)O_4$. As extend Li, Se and O linking, a lithium selenite layer is constructed along the ab-plane. $Mn(SeO_3)_6$ octahedral structures are inserted in these layer and they share O(2) and O(3). Ignoring the Li-O covalent bond, the framework of $Li_{13}M(SeO_3)_8$ is considered as an anionic structure composed of Li^+, SeO_3^{2-} and $[Mn(SeO_3)_6]^{9-}$. Full characterization including thermal analyses, magnetic property measurements and spectroscopic analyses such as electron paramagnetic resonance, Infrared, UV-vis, and X-ray photoelectric spectroscopy will be presented.

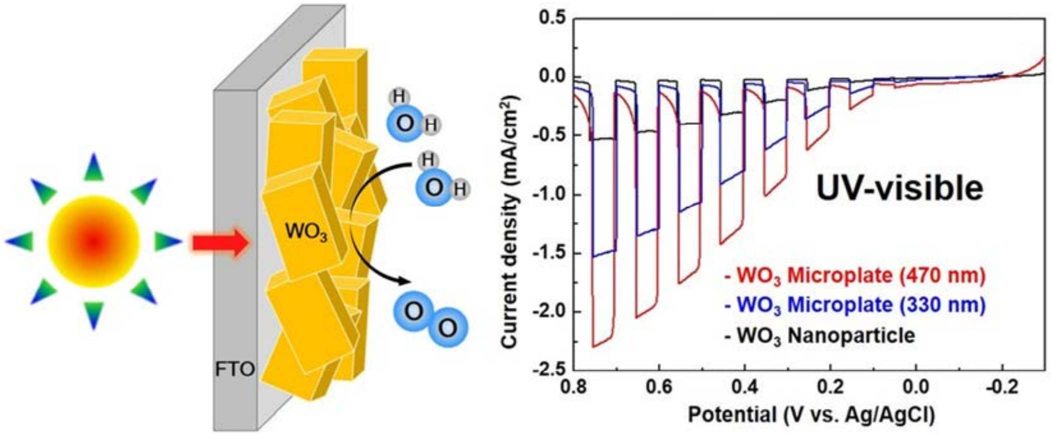
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-97**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of Tungsten Oxide Microplates with High Active in Visible Light for Photoelectrochemical Water Oxidation

박미라 남기민[1,*] 송현준[*]

KAIST 화학과 [1]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. While a multitude of semiconductors have been investigated for potential use in PEC water splitting, the most critical issues are still the development of semiconductors with high photon to charge-carrier efficiency in the visible light region and long-term durability in an aqueous environment. WO3 is an n-type semiconductor, and one of the most promising materials ,however, the relatively low activity in the visible light contributes to the poor overall efficiency for PEC water oxidation. Here we report that a synthesis of single crystalline WO3 on a fluorine-doped tin oxide. The WO3 has a typical microplate shape with perpendicularly oriented to the FTO substrate. The scanning electron microscopy image showed high uniformity of the WO3 microplates and precisely controlled to the average length and thickness only change the concentration of both H2WO4 and oxalic acid. The X-ray diffraction patterns were in good agreement with that of monoclinic WO3 and the relative intensity of the (002) reflection of WO3 microplates electrode is large compared to the reference peak, indicating the coexistence of an oxygen-deficient structure. The PEC performance of the WO3 microplate and nanoparticle electrodes have been studied using linear sweep voltammetry (LSV) in 0.1 M Na2SO4 (pH 7). All electrode samples successfully showed anodic photocurrents, and the microplate with a thickness of 470 nm (MP1) generated 1.9 mA/cm2 at 0.6 V (vs Ag/AgCl) under UV-vis illumination. This result indicate that the thickness of the MP1 was in good agreement with the maximum hole diffusion length, indicating an optimized morphology for effective photogenerated charge separation. Note that the MP1 electrode was better photocurrent under visible light irradiation ($\lambda > 425$ nm) compared to other WO3 electrodes. These enhanced levels of activity mainly originated from the morphology of the single-crystalline domains with an optimum thickness, and the optimized oxygen deficiency of WO3 due to the use of an appropriate annealing procedure.



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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-98**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and optical properties of noncentrosymmetric (NCS) solid solutions, $Ca_4Bi_{6-x}Ln_xO_{13}$ (Ln= Eu and La)

정호용 조홍일 옥강민*

중앙대학교 화학과

$Ca_4Bi_{6-x}Ln_xO_{13}$ (Ln = Eu and La ; x=0.06, 0.12) solid solutions have been synthesized through solid state reactions. The structures of the title compounds were determined by powder X-ray diffraction using the Rietveld refinement. Powder second harmonic generation (SHG) measurements suggest that the host material, $Ca_4Bi_6O_{13}$, exhibits SHG efficiency of 80 times that of SiO_2 and is type-1 phase-matchable. The origin of SHG will be elucidated through the solid solution behavior of the materials. Phtoluminescence (PL) properties and infrared spectra for the solid solutions are also presented.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-99**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Molecular Catalysis of the Photochemical Reduction of CO_2 with Rare and Earth-Abundant Metal Complexes. Selective Production of CO vs HCOOH by Switching of the Metal Center

우성준 김철훈 강상욱 손호진[*]

고려대학교 신소재화학과

In photocatalytic systems for CO_2 reduction, Ru and Re complexes with 2,2'-bipyridine as ligand have been frequently investigated as catalysts. Although several systems with such catalysts showed selective CO_2 reduction with very high efficiency, however they include expensive rare metals. The manganese(Mn) can be alternative metal. Mn is earth abundant transition metal, and Mn is a same group with Re. We investigated the possibility that switching Re complex to Mn complex as a photocatalyst could affect CO_2 reduction. We apply a highly robust hybrid system(sensitizer/TiO_2/catalyst) for the visible-light CO_2 reduction. Studies are reported regarding the use of [Mn(bpy-mPH)$(CO)_3$Br], [Re(bpy-mPH)$(CO)_3$Cl] as a catalyst for CO_2 reduction OrgDH as a photosensitizer in mixtures of dry N,N-DMF with BIH as a sacrificial reductant. In this study, the Mn complex showed the best activity visible light conditions, giving a high TN_{HCOOH} of >250 during 30 h, while Re complex revealed the best activity visible light conditions TN_{CO} of >150 during 30 h under ≥ 420 nm 3 LED lamp irradiation and Merry-go-round type reactor conditions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-100**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Nature-inspired, Highly Efficient CO_2 Reduction System Consisting of Red Absorbing Porphyrin Trimers

최성한 김철훈 강상욱 손호진*

고려대학교 신소재화학과

Photocatalytic systems for CO_2 reduction using butadiyne-linked porphyrin trimers and dimers as sensitizers were investigated. ReC, (4,4′-bis(methylphosphonic acid)-2,2′-bipyridine)ReI$(CO)_3$Cl as the catalyst, was anchored on TiO_2 particles through the methylene-bridged phosphonic acid substituents of the bipyridine ligand for the construction of binary systems. In this study, the porphyrin dimer based system showed the best activity under low-energy light conditions, giving a high TN_{CO} of >270 during 3000 min, while porphyrin trimer based system revealed the best durability because of wavelength variation, showing no leveling-off tendency for >50 h to give TN_{CO} of ~400.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-101**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Highly Selective Photocatalytic Reduction of CO_2 using Red Light absorbing squaraine sensitizers

조민지 김철훈[1] 강상욱 손호진[*]

고려대학교 신소재화학과 [1]고려대학교 세종캠퍼스 신소재화학과

Recently, the photochemical and photoelectrochemical reduction of CO_2 has grown rapidly in the last few decades. As a role model, natural photosystem has only used the limited region (red light) among visible light for light-harvesting with efficient blue light protection by carotenoids (as carotenoids absorb blue light), functioning as photoprotectants in photosynthesis. Therefore, low-energy photo-sensitization is a key issue in the realization of solar light harvesting for highly efficient artificial photosynthesis systems and solar cells. The introduction of efficient red light absorption dye is very essential (desirable) to build an efficient artificial photosynthetic system with obtaining its long-term durability. Squaraine dyes are one of the most promising candidates owing to their high extinction coefficients in NIR region (600-800 nm) and easy synthetic route. Herein, we present the detailed characterization and principles of ternary system (sensitizer/TiO_2/Re(I)) for CO_2 reduction, which is constructed by the covalent anchoring of both a red light active squararine (sensitizer) and a Re(I) complex catalyst (RePH) on metal oxide particles. We found the photocatalytic efficiencies were found to be substantially affected by the anchoring group and quality of semiconductor, water content in the solvent on the photocatalytic activity of the hybrid particles. This study also includes some interesting findings from the structural modification of squaraine sensitizer and the spectral range control of irradiated light source that influence the long-term stability of overall photocatalytic system.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-102**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Visible-Light driven Photoreduction of CO_2 with Zn-Porphyrin based Metal Organic Frameworks (MOFs) as Highly Stable Photosensitizer

김필수 김철훈 강상욱 손호진*

고려대학교 신소재화학과

Porphyrin based metal-organic frameworks (MOF) (PCN-222) coupled with a Re(I) molecular catalyst selectively reduced CO_2 into CO under visible light ($\lambda > 400$ nm) in the presence of a suitable electron donor with high durability. Modification of PCN-222 with post TiO_2 ALD coating resulted in a PCN-222/TiO_2/Re(I) hybrid catalyst exhibiting a very steady catalytic activity (a turnover number of >150 with respect to the amount of Re(I) catalyst), while maintaining high selectivity for CO production (>98%). This turnover number is 30 times higher than that reported previously using MOF modified with a mononuclear Ru(II) complex, and by far the highest among the hybrid systems with combination of MOF and Re(I) catalyst reported to date. The results of photocatalytic reactions, emission decay measurements, and time-resolved absorption spectroscopy shows that TiO_2 ALD layer coated on PCN-222 collects efficiently the photo-excited electrons of Zn-porphyrin units in PCN-222, which were transferred to Re(I) catalytic site, thereby promoting photocatalytic CO_2 reduction driven by net electron transfer from TiO_2 layer to the immobilized Re(I) site. By using this photocatalytic system, CO_2 of 1 and 10% concentration could be selectively converted to CO with almost same performance to that under a 100% pure CO_2 atmosphere, reflecting the effective integration of CO_2 capture by MOF.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-103**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Influence of the Second-Phase Intercalation on the Thermoelectric Properties of the Zintl Phase $Ca_{1.5}Yb_{3.5}Al_2Sb_6$:AlSb/ InSb

최웅진 유태수*

충북대학교 화학과

Thermoelectric (TE) materials can be used to transfer the wasted heat from many different heat sources into electricity via the Seebeck effect. Among various candidate materials, Zintl phase compounds are one of the attractive choices for TE application due to their intrinsically complex crystal strurctures and semiconducting characteristics. In particular, a Zintl compound $Ca_{1.5}Yb_{3.5}Al_2Sb_6$, which is a member of the the solid-solution $Ca_{5-x}Yb_xAl_2Sb_6$ ($1.0 \leq x \leq 5.0$) system including a mixed cation of Ca^{2+} and Yb^{2+}, has shown a significantly enhaced ZT value as the structure type transformed from the $Ba_5Al_2Bi_6$ to the $Ca_5Ga_2Sb_6$ after annealing treatment for a month. Two slightly differnet crystal structures of the $Ba_5Al_2Sb_6$-type and $Ca_5Ga_2Sb_6$-type phases were characterized before and after annealing, respectively, by both powder and single-crystal X-ray diffraction analyses. The two title phases adopt the orthorhombic space group *Pbam* (Z = *2*, *oP*26). To further enhance ZT value of this Zintl compound, we have attempted to introduce a small amount of a second phase, such as AlSb and InSb, which can act as a phonon scatter and increase the electrical transport property. Thus, two binary compounds acting as a secondary phase, respectibvely, were pre-synthesized, then mixed with other elements to produce the targeted mixed-compound of $Ca_{1.5}Yb_{3.5}Al_2Sb_6$ and AlSb or InSb. A series of physical property measurements, including electrical conductivity, Seebeck coefficient, and thermal conductivity, were conducted. In addition, 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 of the title compounds.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-104**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Properties of Ruthenium Nitrosyl Complexes with Schiff base ligand

김민영 이홍인* 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, ruthenium nitrosyl complexes have been proposed as attractive photodynamic therapeutic agents in biomedicine and in tumor treatment. This research aims at developing ruthenium nitrosyl complexes which absorb long wavelength visible light to release NO with high quantum yield. 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 progress with modified Schiff-base ligands to increase the solubility of the ruthenium complexes in water and the properties of NO-releasing of the complexes monitored by UV-VIS, IR spectroscopy, EPR.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-105**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Selective Reduction of CO_2 Using 2-Component Hybrid System (Ir-Ps + TiO_2/ReC): Effects of Electronic Structure control on Cationic Ir-Complexes

정하연 김철훈 강상욱 손호진*

고려대학교 신소재화학과

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 = ^{t}Bu ~ Me > OMe > 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 $Ru(bpy)_2^{2+}$, a widely used transition-metal photosensitizer and (2) the system comprising Ir-^{t}Bu^+ and TiO_2/ReC is much more efficient than a homogeneous-solution system using Ir-^{t}Bu^+ 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: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-106**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

질소가 도핑 된 활성탄을 이용한 금속이온 흡착

김동관 김희수 정희승 유원철*

한양대학교 응용화학과

Cu, Fe, Zn 등과 같이 수질 속 미량 존재하는 인체에 유해한 금속이온을 제거하기 위한 방법으로, 화학적 처리를 통하여 제거할 때에는 미량의 금속이온 제거가 어려울 뿐 아니라 화학적 처리를 위해 화학약품을 사용해야 한다. 이 경우 응집에 사용된 잔여 화학물질로 인한 오염이 발생할 수 있고, 이러한 이유로 화학물질을 사용하지 않고, 효과적으로 수질 속 금속이온을 제거 할 수 있는 흡착제의 개발이 필요하다. 이러한 이유로 인하여 화학 약품을 사용하지 않고 수질 속 금속이온을 효율적으로 제거하기 위해 전구체로서 고분자 이용하여 구형 탄소를 제조하고, CO_2 활성화 과정을 통하여 구형 탄소의 기공특성 (표면적, 기공부피 등)을 조절하고 금속이온 흡착능과의 상관관계에 대한 연구를 진행하였다. 처음으로, Resorcinol 과 Formaldehyde 를 이용해 RF Polymer 를 합성한 후 탄화 과정을 진행하여 RF Carbon (RFC)을 제조했다. 이렇게 만들어진 탄소의 Porosity 를 향상시키고, Porosity 증가와 흡착성능 사이의 관계를 조사하기 위하여 CO_2 활성화 과정 ($C+CO_2$ -> 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 흡착성능이 상승하는 경향성을 나타냈다. 또한 구형의 탄소물질의 Polarity 가 금속이온 흡착능에 미치는 영향을 조사하기위해 질소를 함유한 Dopamine hydrochloride 을 전구체로 이용하여, Melanin Polymer 를 합성한 후 탄화과정을 통해 질소가 도핑된 Melanin Carbon (MC) 을 제조하였다. CO_2 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 동일한 Porosity 에서 질소가 도핑된 MC 활성탄의 금속 흡착능이 RFC 활성탄 보다 더 높은 것을 확인할 수 있다. 구형 탄소물질의 Porosity 가 증가 할수록 물리적인 흡착성능의 증가로 인해 수질 속 금속이온의 제거 효율이 높아지고, 동일 Porosity 를 가지는 물질 중 Nitrogen

도핑으로 Polarity 가 증가 된 물질의 경우 물리적인 흡착 뿐만이 아닌, 금속이온과의 화학적 흡착으로 인해 더 높은 흡착능을 보여준다.

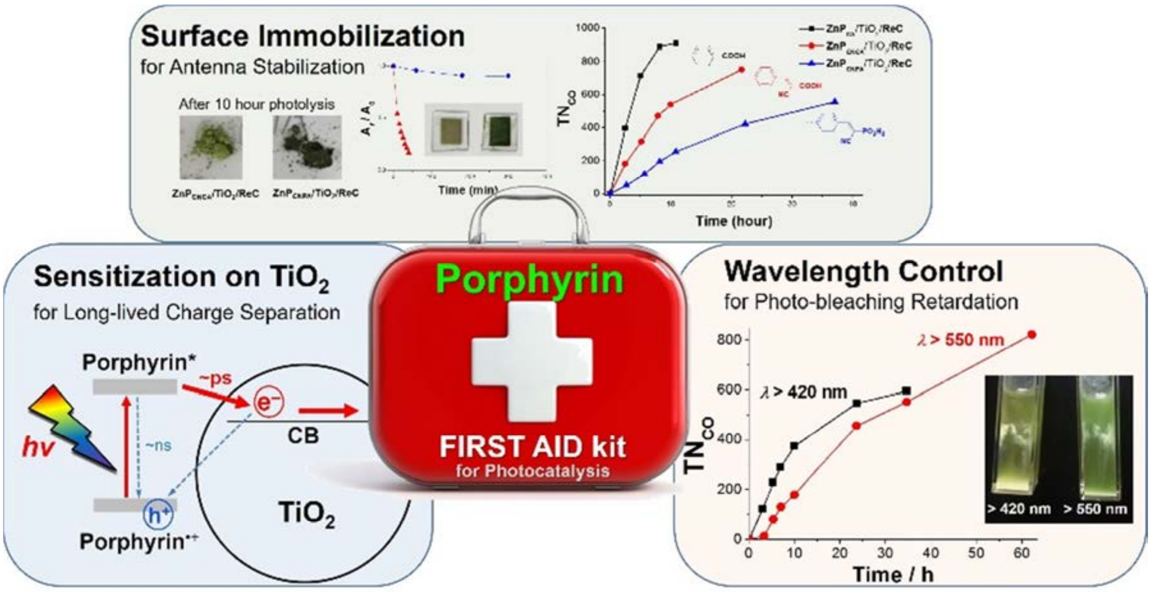
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-107**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High Performance Photocatalytic CO_2 Reduction by Low Energy Sensitization

원동일 김철훈 강상욱 손호진*

고려대학교 신소재화학과

Porphyrin dye was chosen to test 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 relate to the steady performance on the photocatalytic CO_2 reduction. Three appropriate anchoring groups (-COOH (ZnP_{CA}), -CNCOOH (ZnP_{CNCA}), -$CNPO_3H_2$ (ZnP_{CNPA})) were combined with the porphyrin ring in order to examine the anchoring group effects on the porphyrin light harvester. A series of visible light sensitizing porphyrin antenna have been engaged to the hybrid photocatalyst system for CO_2 reduction and recorded unprecedented catalytic performance. The photocatalytic activities are dramatically increased in the order of $ZnP_{CA} > ZnP_{CNCA} > ZnP_{CNPA}$, whereas longevities follow in reverse order ($ZnP_{CA} < ZnP_{CNCA} < ZnP_{CNPA}$), implying a direct anchoring group-dependency in the photochemical CO_2 reduction. In this study, the ZnP_{CA}-based hybrid system showed the best activity under low-energy light conditions, giving a high TN_{CO} of >1000 during 40 h, while ZnP_{CNPA}-based catalytic system revealed the best durability irrespective of wavelength variation, showing no leveling-off tendency for >90 h to give TN_{CO} of ~800.


Surface Immobilization
for Antenna Stabilization
After 10 hour photolysis
ZnP/TiO2/ReC
A / A0
Time (min)
TNCO
Time (hour)
ZnP/TiO2/ReC
COOH
PO3H2
Porphyrin
FIRST AID kit
for Photocatalysis
Sensitization on TiO2
for Long-lived Charge Separation
Porphyrin*
~ps
e⁻
CB
hv
~ns
h⁺
Porphyrin•+
TiO2
Wavelength Control
for Photo-bleaching Retardation
λ > 550 nm
λ > 420 nm
TNCO
Time / h
> 420 nm
> 550 nm

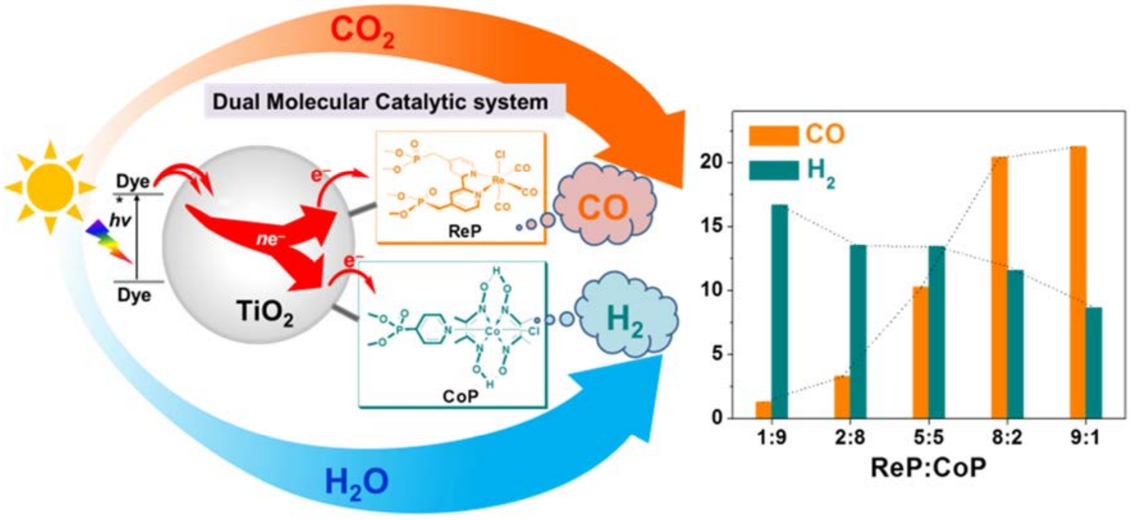
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-108**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Selective Syngas (H_2 + CO) Production through Immobilized Dual Molecular Re(I)^{I}/Co^{III} Catalyst on a Dye-Sensitized TiO_2 Hybrid System under Visible-Light Irradiation

원동일 강상욱 손호진*

고려대학교 신소재화학과

Visible-light irradiation of a ternary hybrid catalyst prepared by grafting a dye, a H_2 evolving Co(III) catalyst and a CO-producing Re(I) catalyst on TiO_2 produced both H_2 and CO (syngas) in CO_2-saturated DMF/water solution containing 0.1 M SED (sacrificial electron donor). The H_2/CO ratios are effectively controlled by changing either the water content in solvent (0 to 20 vol%) or the molar ratio of the Re(I) and Co(III) catalysts to the ratios of from 1:9 to 9:1 and further to the ratios being from 1:2 to 15:1. The controlled syngas formation is observed from the assumption that there exist competitive electron flow passages from TiO_2 to each of the CO_2-reduction and hydrogen-evolving sites. We have found that depending on the efficiencies of the two catalytic reaction cycles under given reaction conditions, syngas composition varies greatly; CO_2 solubility in the solvent and further solubility variation by added water content are the prime factor; the amount of CO evolved during the reaction interferes authentic catalytic cycle that CoP complex carries on for catalytic hydrogen production. Complete picture of photocatalytic syngas production will be presented.


CO₂
Dual Molecular Catalytic system
Dye*
hv
Dye
TiO₂
ne⁻
e⁻
e⁻
ReP
CoP
CO
H₂
H₂O
CO
H₂
0
5
10
15
20
1:9
2:8
5:5
8:2
9:1
ReP:CoP

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-109**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Logical Inference on MOF Structure Based on Its Growth Behavior and Morphological Feature

최소라 오문현*

연세대학교 화학과

The integration of metal-organic framework (MOF) with different kind of MOF to form hybrid MOF containing more than two kinds of MOFs in one particle is a central goal in the MOF development because the management of the composition and structure of MOF is essential for fine tuning their properties. However, there are only few examples for understanding the hybrid MOF formation through the growth of MOF on MOF. Herein, we report the investigation of the isotropic and anisotropic growth of two MOFs, named MIL-68-Br and MOF-NDC, on a micro-sized MOF template made from MIL-68. The isotropic growth of MIL-68-Br on the MIL-68 template resulted in the core-shell type MIL-68@MIL-68-Br. However, the fascinating anisotropic growth of MOF-NDC on the MIL-68 template resulted in the formation of unusual semi–tubular particles. The crystal structure of a new MOF (MOF-NDC) was speculated based on its unique growth behavior and morphological features and the speculated MOF structure was validated from powder X-ray diffraction and selected area electron diffraction studies.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-110**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Metal-Organic Framework Particles for Tunable White Light Emission

박지현 오문현*

연세대학교 화학과

White-light-emitting diodes (WLEDs) have attracted great attention due to their many useful applications in backlighting, illumination, indicators, and displays. White phosphor materials can be prepared from various materials including organic molecules, metal complexes, organic-inorganic hybrid materials, quantum dots, and metal-organic frameworks (MOFs). Among them, MOFs are fascinating materials used to construct excellent white phosphor materials since a broad range of luminescent metal ions and organic linkers can be used for the MOF fabrication. Herein, we report the synthesis of micro-sized white-light-emitting MOF particles fabricated from blue-emitting organic linker, and red- and green-emitting lanthanide ions(III). The amounts of the three different components, a pyrene-based organic linker for blue emission, Eu^{3+} for red emission, and Tb^{3+} for green emission, were adjusted to achieve good white light emission.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-111**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Syntheses, crystal structures, and properties of dinuclear iron(III) and nickel(II) complexes with *N*-(2-pyridylmethyl)-*N´*-(2-hydroxyethyl)ethylenediamine

정아림 민길식[1,*]

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Dinuclear iron(III) and nickel(II) complexes, $[(\text{phenO})\text{Fe}^{\text{III}}(N_3)]_2$ (**1**) and $[(\text{phenOH})\text{Ni}(N_3)_2]_2$ (**2**) have been prepared by the reaction of phenOH, NaN_3 and $Fe(NO_3)_3{\bullet}9H_2O/Ni(NO_3)_2{\bullet}6H_2O$ in methanol, respectively (phenOH = *N*-(2-pyridylmethyl)-*N´*-(2-hydroxyethyl)ethylenediamine). The dinuclear complexes have been characterized by elemental analysis, IR spectroscopy, X-ray structural analysis, and magnetic susceptibility measurement. Two iron(III) ions in **1** are ethoxo-bridged, while two nickel(II) ions in **2** are azido-bridged. Each metal ion in **1** and **2** has six-coordinated in distorted octahedral geometries. **1** shows an antiferromagnetic interaction through the bridged ethoxo groups within the dimeric unit, while **2** displays a strong ferromagnetic coupling through the bridged end-on azido ligands in the dimer. The catalytic activities of **1** and **2** have been investigated for olefin epoxidation reactions. No catalytic activity in **1** is observed. However, **2** shows excellent catalytic activities for olefin epoxidations and terminal olefin epoxidations as a homogenous catalyst. In this poster, we will present the detailed preparation of the ligand and iron/nickel compounds, crystal structures, and properties.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-112**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Study on crystal structures and magnetic properties of two dinuclear nickel(II) complexes with *N*-(2-pyridylmethylamino)-2-methylpropan-1-ol

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We have synthesized two nickel(II) complexes, $[(pmapO)Ni(N_3)_2]_2 \cdot MeOH$ (**1**) and $[(pmapO)_2Ni_2(OAc)(N_3)_3]$ (**2**), containing *N*-(2-pyridylmethylamino)-2-methylpropan-1-ol (pmapOH) ligand which has one pyridine, one amine, and one hydroxyl group. The nickel(II) complexes were characterized by IR spectroscopy, single crystal X-ray diffraction. In **1**, two nickel(II) ions are each coordinated with two N atoms and an O atom of the $pmapO^-$ ligand and three N atoms from azide anions. In **2**, one nickel(II) ion is coordinated with two N atoms and an O atom of the $pmapO^-$ ligand and three N atoms from azide anions, the other nickel(II) ion is coordinated with two N atoms and an O atom of the $pmapO^-$ ligand and an O atom from acetato ligand and two N atoms from azide anions. Both **1** and **2** show ferromagnetic interactions between the nickel(II) ions. In this poster, we will explain the detailed preparation of the ligand and nickel(II) complexes, crystal structures, and magnetic properties.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-113**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A Dye-Sensitized Photoanode based Tandem Cell for Best Performance of Water Splitting

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Tandem junction photoelectrochemical watersplitting devices, whereby two light absorbing electrodes targeting separate portions of the solar spectrum generate the voltage required to convert water to oxygen and hydrogen, enable much higher possible efficiencies than single absorber systems. We report here on the development of a tandem system consisting of a dye-sensitized photoelectrochemical cell (DSPEC) wired in series with a dye-sensitized solar cell (DSC). The DSPEC photoanode incorporates a tris(bipyridine)ruthenium(II)-type chromophore and molecular ruthenium based water oxidation catalyst. The DSPEC was tested with two more-red absorbing DSC variations, one utilizing N719 dye with an I_3^-/I^- redox mediator solution and the other D35 dye with a tris(bipyridine)cobalt ($[Co(bpy)_3]^{3+/2+}$) based mediator. The tandem configuration consisting of the DSPEC and D35/$[Co(bpy)_3]^{3+/2+}$ based DSC gave the best overall performance and demonstrated the production of H_2 from H_2O with the only energy input from simulated solar illumination.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-114**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Pseudo-Polyrotaxane Architecture with *String* and *Bead* Consisted of the Same Components

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1D + 2D → 3D *Pseudo*-polyrotaxane constructed by the penetration of 1D coordination polymer chains into 1D channels formed by parallel stacking of 2D porous coordination layers is a quite rare topology. Until now, only a few examples of 1D + 2D → 3D *pseudo*-polyrotaxanes have been reported and their 1D chains and 2D sheets acting as the *strings* and the *beads*, respectively, are made up of different components each other.

In this presentation, we present a scarcely rare 3D pseudo-polyrotaxane whose *string* and *bead* are made up of same compositions. The 3D *pseudo*-polyrotaxane, namely $\{[\mathrm{Ag}(\mathbf{L})][\mathrm{Ag}_2(\mathbf{L})_2]\cdot(\mathrm{BF}_4)_3\cdot(\mathrm{CH}_3\mathrm{CN})_2\}_n$ (**1**), is obtained by the self-assembly of AgBF_4 with a dipyridyl-type ligand *N*-(pyridine-3-ylmethyl)pyridine-3-amine (**L**) in acetonitrile.[1] The 3D *pseudo*-polyrotaxane **1** is topology constructed by 1D $[\mathrm{Ag}(\mathbf{L})]_n$ chains (*strings*) threading through cavities generated by parallel stacking of honeycomb-like 2D $[\mathrm{Ag}_2(\mathbf{L})_2]_n$ layers (*beads*) in 1D + 2D → 3D fashion. Intermolecular π-π stacking and cation···π interactions between the strings and the beads between contribute to the stabilization of the 3D *pseudo*-polyrotaxane. Furthermore, the tetrafluoroborate anions promote the formation of 1D + 2D → 3D *pseudo*-polyrotaxane through N/C-H···F hydrogen bonds.

[1] H. Im, E. Lee, S.-H. Moon, S. S. Lee, T. H. Kim, K.-M. Park, *Bull. Korean Chem. Soc.* **2017**, *38*, 127-129.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-115**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Direct conversion of coordination compounds into Ni2P nanoparticles entrapped in 3D mesoporous graphene for efficient hydrogen evolution reaction

정성은 서보라[1] 주상훈[2] 문회리[1,*]

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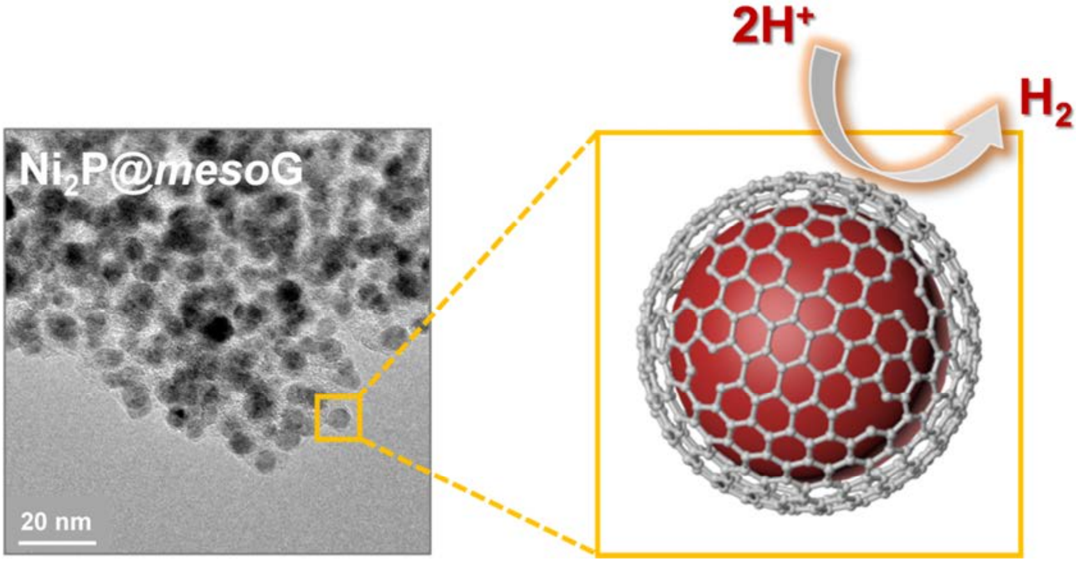
This paper reports a simple preparation route for the composite of small Ni2P NPs entrapped in 3D mesoporous graphene by the thermal conversion of a coordination compound and the followed phosphidation. Recently, transition metal phosphides (TMPs) have gained increasing attention, owing to their promise as non-precious metal catalysts in HER. In order to enhance the catalytic activity of TMPs, researchers have sought to synthesize small TMP NPs to increase catalytically active surface area. Although surfactant-mediated syntheses can produce small TMP NPs, a cumbersome surfactant removal step is necessary to generate catalytically active clean surfaces. Interfacing TMP NPs with carbon nanomaterials is another promising approach to boost the catalytic performance by providing high electrical conductivity and durability. However, the synthesis of composites of TMP NPs and carbon demands multiple synthetic steps, including the preparation of TMP NPs, synthesis of carbon nanomaterial, and dispersion of TMP NPs onto the carbon support. The essence in our approach toward the 3D graphene encapsulating Ni2P NPs (Ni2P@mesoG) lies in the utilization of the conversion phenomenon of [Ni2(EDTA)]. The thermolysis of [Ni2(EDTA)] at 600 °C produces a composite of single-crystalline 5 nm-sized Ni NPs individually entrapped in 3D mesoG, and the following phosphidation completely converts it to single-crystalline Ni2P NPs in mesoG (Ni2P@mesoG) without agglomeration. Notably, graphitic shell layers in Ni2P@mesoG stabilize small Ni2P NPs possessing a large active surface area, and facilitate the electron transfer due to the intimate contact between them. Consequently, the use of Ni2P@mosoG exhibits superior electrocatalytic HER activity and durability in both strong acidic and basic media.


Ni2P@mesoG
20 nm
2H+
H2

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-116**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Zn_2SnO_4 Particles Coated with N-doped Carbon as an Anode Material for Lithium-Ion Batteries

김남영 김한아 김종식*

동아대학교 화학과

Lithium-ion batteries (LIBs) have been widely used in broad application such as mobile devices, electric vehicles, and hybrid electric vehicles. However, LIBs are still required to improve discharge capacity, electronic conductivity, and cycle life in spite of several benefits such as high power density and high energy density. Graphite is currently commercialized as anode material in LIBs. Nevertheless, researches are still needed on exploring alternative anode materials in place of graphite because of its slow diffusivity for lithium ions and low instinct capacity of about 372 mAh g^{-1}. Zinc stannate (Zn_2SnO_4) can be one of the promising anode materials for LIBs due to its high discharge capacity of about 1231 mAh g^{-1}. However, Zn_2SnO_4 have drawbacks of its large volume changes during the insertion and extraction processes of lithium ion, resulting in particle pulverization and poor cycling stabilities on repeated cycles. In this study, these problems are alleviated by coating N-doped carbon on Zn_2SnO_4 particles. Zn_2SnO_4/N-doped carbon (Zn_2SnO_4/NC) composites were synthesized by a facile hydrothermal reaction using dopamine as both carbon and nitrogen sources. The Zn_2SnO_4/NC exhibited the enhanced electrochemical performance with the initial discharge capacity of about 1251 mAh g^{-1} and a capacity fading rate of about 0.43% per cycle during the 2-50 cycles at current density of 60 mAg^{-1} in the voltage range of 0.005-3.0 V, which is superior those of bare Zn_2SnO_4.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-117**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Activation of C–H Bonds in Metallocenium Cations by N-Heterocyclic Carbenes as an Effective Route to Two-electron Redox Metallocene-NHC Cationic Complexes

전승원 이은성*

POSTECH 화학과

Activation of carbon–hydrogen bonds in ferrocenium cations by N-heterocyclic carbenes (NHCs) has been demonstrated as an effective route to access two-electron redox ferrocene NHC cationic complexes. The ferrocene NHC cations were applied to one-electron reduction and oxidation reactions to afford neutral ferrocene NHC radical and biscationic ferrocenium NHC complexes, respectively. The ferrocene NHC cationic complexes, thus, can be used as two electron redox standard compounds with a good tunability depending on the choice of NHC. These investigations of the unique reactivity of NHC toward metallocenium cations will certainly prove valuable for gaining our basic understanding towards the intrinsic reactivity of NHCs.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-118**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Hierarchical $Ni_{3.5}Co_{5.5}S_8$ hollow nanocages: Superior electrocatalyst towards oxygen evolution reaction

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Developing highly efficient and cost-effective electrocatalysts for oxygen evolution reaction (OER) is crucial for renewable energy storage technologies. Here, we synthesized hierarchical Co-based bimetallic sulfide nanostructures as an efficient electrocatalyst for OER. $Ni_{3.5}Co_{5.5}S_8$ nanostructures were synthesized by solvothermal sulfurization and thermal annealing of pre-synthesized homogeneous bimetallic metal-organic frameworks (MOFs). Electron microscopy studies revealed that the $Ni_{3.5}Co_{5.5}S_8$ has hollow nanocage morphology with thin nanosheets grown on the surface. The $Ni_{3.5}Co_{5.5}S_8$ hierarchical nanostructures has exhibited a low overpotential of 333 mV at the current density of 10 mA cm^{-2} and Tafel slope of 48.5mVdec^{-1} for the oxygen evolution reaction in 1M KOH. Benefitting from their structural merits, $Ni_{3.5}Co_{5.5}S_8$ has excellent electrocatalytic activity towards OER.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-119**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and optical properties of Au-Cu intermetallic nanoparticles: an systematic approach on complex dielectric function via spectroscopic method and theoretical model

<u>오현철</u> 박영찬 류설[1,*] 송현준[*]

KAIST 화학과 [1]조선대학교 화학과

An analytical development on the optical properties of alloy nanoparticles enable a variety of applications by tuning their plasmon resonance. However, a composition-weighted linear-combination of complex dielectric function does not account for realistic results of alloys. Herein, we introduce a new approach to analyze the optical properties of the alloy nanoparticles using Au-Cu intermetallic nanoparticles. As a well-known intermetallic system, Au-Cu nanoparticles are suitable to study the complex dielectric function in detail via the correlation between experimentally obtained results and those predicted by theory. We analyzed the complex dielectric function of Au-Cu intermetallics measured by variable angle spectroscopic ellipsometry (SE) using the theoretical results calculated by density functional theory (DFT). From these results, we found that Au-Cu nanoparticles show non-linear shift of plasmon peak position with increasing of Cu contents.Abnormal behavior of complex dielectric function of Au-Cu intermetallics, compared to other alloys, can be resulted from damping frequency and electron mean free path according to the previous reported studies. The obtained dielectric function is used to calculate the extinction efficiency using finite-difference time-domain (FDTD) method. These calculated plasmon peaks are well correlated with the peak positions measured by single-particle dark-field spectroscopy. This work can be expanded to other plasmonic alloy systems for improving our understanding on the desirable optical properties.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-120**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, crystal structure, and physical properties of a 3D manganese-based metal-organic framework

이한글 송정화 강동원 이화영 강민정 김정은 엄선휘 홍창섭*

고려대학교 화학과

We have synthesized a three-dimensional manganese-based metal-organic framework $[Mn_4(H_2L^{2-})_2(L^{4-})(MeOH)_2(DEF)]$(1) (L = 2,3-dioxido-1,4-benzenedicarboxylate) via a solvothermal reaction. We used $MnCl_2 \cdot 6H_2O$ as a central metal and H_4L (2,3-dioxido-1,4-benzenedicarboxylic acid) as an organic linker in a mixed solvent of DEF and MeOH. Compound 1 crystallizes in the monoclinic system with the space group C2/c. Compound 1 was characterized by single crystal X-ray diffraction, powder X-ray diffraction, elemental analysis, and IR. Detailed structure and other measurements will be given in the presentation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-121**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

다양한 인듐계 발광체의 합성과 광학 특성연구

우원희 현경림 곽상우 이강문[1] 박명환[2,*] 김영조[*]

충북대학교 화학과 [1]강원대학교 화학과 [2]충북대학교 화학교육과

13 족 금속인 알루미늄과 갈륨 기반 유기금속 화합물들은 열적 안정성과 광물리적 특성이 우수하여 있어 광전자 소재로 널리 이용되어 왔다. 반면에 인듐계 유기금속 발광체에 대한 연구는 거의 알려져 있지 않다. 본 연구에서는 Schiff base 기반 다양한 신규 인듐 화합물을 합성하고 NMR 및 X-선 단결정 실험 분석을 통하여 그 구조를 규명하고, UV/vis, PL 측정 실험을 통하여 합성된 각 화합물들의 발광 특성에 대하여 발표하고자 한다.Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

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장소: 일산 KINTEX
발표코드: **INOR.P-122**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Microstructured and Adhesive Organic Network Films: Useful Platforms for the Engineering of Flexible Current Collectors*

강창완 최재원 손성욱*

성균관대학교 화학과

This presentation will show the synthesis of microstructured and adhesive organic network films (MONF) and their application for the engineering of flexible current collectors. Flexible energy storage devices have attracted the recent attention of scientists due to the needs of wearable devices. As an essential component of flexible energy storage devices, the flexibility of current collectors is important. Although carbon materials and conducting polymers have been applied for the engineering of flexible current collectors, their relatively low conductivities are drawbacks. In this regards, metal-polymer composites are attractive due to excellent conductivities. The organic network films have flexibility and thus, can be applied as chemical components of flexible devices. Using the assembled silica zeolite bricks with 2D morphology as templating materials, microstructured organic network films with hollow space were prepared through the Sonogashira coupling of tetrakis(4-ethynylphenyl)methane and 1,4-diiodobenzene and successive silica etching. Interestingly, the MONF has regular holes on the bottom and thus, was tightly adhered to PET film. We speculate that the unique hole structure of MONF induced tight attachment to PET film, resembling the sticky performance of octopus legs towards solid supports. The Cu was deposited on the MONF/PET through electroless deposition. The Cu/MONF/PET showed excellent conductivity retention against the repeated bending actions. In contrast, Cu on the PET films was easily detached and showed the gradual decrease of conductivity in the repeated bending actions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-123**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Introduction of BL2D-Supramolecualr Crystallography Beamline Performance Upgrade

김대웅 문도현*

포항가속기연구소 빔라인운영부 생명화학구조팀

포항가속기연구소 초분자 결정학 빔라인(Supramolecular Crystallography Beamline; BL2D-SMC)은 방사광 가속기를 이용한 국내 유일의 단결정 결정학 실험 시설로서 유기 무기 소형 분자 및 초분자 단결정 구조분석 실험 장치이다. 방사광에서 발생되는 다양한 에너지 가운데 1.5~0.6 Å 의 단파장을 선택적으로 사용가능하며, 85~500K 온도 변화 및 기체 흡착 등 외부 실험 장치를 이용한 다양한 구조 분석이 가능하다. 이러한 장치들은 빔라인 소프트웨어(BL2D-SMCD)를 통하여 이용자가 쉽게 조정 및 사용 할 수 있다. 새로운 온도 장치인 Cryojet 5 를 이용하면, 기존보다 8 배 빠른 온도 변경이 가능하다. 또한, 2017 년 말 설치 예정인 초고속 검출기 (Rayonix MX225HS CCD) 및 10 Gbps 네트워크 시스템을 이용하게 되면, 이전보다 최대 10 배 이상의 고속화 실험을 통하여 새로운 단결정의 구조 변화 현상에 대한 실험이 가능할 것으로 생각된다. 본 포스터를 통하여 포항가속기연구소의 초분자 결정학 빔라인의 장치 및 성능향상에 대한 소개를 하고자 한다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-124**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of ternary sulfide and its application toward hydrogen evolution reaction

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고려대학교 화학과

Hydrogen energy is one of the most prospective alternative energy sources, due to its sustainability and high efficiency. Nowadays, transition metal sulfide materials have received great attention due to their intrinsic nature such as metallic properties and structural robustness. Herein, we introduce a simple synthetic method for ternary sulfide nanostructure which is robust enough to withstand a harsh acidic condition during the hydrogen evolution reaction (HER). We could synthesize mixed metal sulfide nanostructures which show superior electrocatalytic activity toward hydrogen evolution reaction.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **INOR.P-125**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of quaternary yolk-shell nanostructures toward bifunctional electrocatalysts in water splitting

하동선 박종식 이광렬*

고려대학교 화학과

The development of bifunctional electrocatalysts with a excellenct reaction kinetics toward both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) is one of the critical goals in electrocatalyst research. Iridium and platinum have been the best performing catalyst in OER and HER, respectively. Herein, we show the preparation of quaternary nanostructures with Pt-based yolk-Ir based shell by fine controlling the reaction kinetics as well as their excellent bifunctional electrocatalytic activity toward OER and HER.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

One-step PtM alloy hetero-structure by using different decomposition kinetics of metal precursors

권혁부 박종식 이광렬*

고려대학교 화학과

Certain noble metals, especially platinum, are well known for their superior activity in electrocatalysis reactions. But their scarcity and high price limit their usage in industrial scale. Therefore, there has been a huge need in researches to develop efficient catalysts with high catalytic activity while using less amount of noble metals.Alloying with non-precious metals is one of the promising strategies for cost reduction. In particular, Pt–Ni and Pt-Cu alloys have attracted a particular interest as promising ORR catalysts owing to their higher activity than that of any other Pt–M compositions. Herein, we report one-pot synthesis of novel PtM hetero-nanostructures which consist of inner dendritic core and outer shell. They show enhanced ORR activity and stability compared to commercial Pt/C.

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Synthesis of ternary alloy nanoframes with nanoscale compositional control with enhanced electrocatalytic activity and durability

전민기 권태현 이광렬*

고려대학교 화학과

Formation of noble metal hollow nanostructures such as nanocages and nanoframes gives electrocatalytic robustness and enhanced activity due to their intrinsic high surface-to-volume ratio. Herein, we suggest that a simple synthetic strategy to prepare alloy nanoframe with nanoscale compositional control in order to enhance the stability of hollow nanostructures. Specifically we prepared compositionally supported nanoframes, PtCu nanoframes with PtCo skin. Furthermore, the thickness of resulting nanoframe structure is easily controlled by simple kinetic control during the nanostructure formation process.

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Facile synthetic route to nanoframe by passivating the exposed facet through lanthanide element and its electrocatalytic application toward oxygen evolution reaction

홍용주 진하늘 이광렬*

고려대학교 화학과

Noble metal-based multi-metallic nanocatalysts have shown a great potential for electrocatalytic oxygen evolution reaction (OER). Hetero-atomic frame nanostructures received a considerable attention due to their large surface area and optimum surface electronic structure. Recently, we found a facile route to form frame nanostructures by aid of lanthanide elements which passivate the exposed facets and induce the growth of iridium mainly on the edge side of template. We have successfully synthesized IrNi alloy nanoframe via the assistance of lanthanide elements. These frame structures exhibit enhanced electrocatalytic performance toward OER.

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Ternary Ir-based octahedral nanocages for efficient water splitting catalyst

권태현 이광렬*

고려대학교 화학과

Development of electrocatalysts with reduced noble metal content and enhanced catalytic performance has been of importance in cost-effective design of acid polymer electrolyte membrane water electrolyzers and fuel cells. Hollow nanostructures with inherently high surface area, in particular, have been actively pursued due to the expected cost-effectiveness. Iridium-based nanostructures are widely used as electrocatalysts toward oxygen evolution reaction (OER), which is the key reaction for water splitting process. However, Ir-based catalysts with well-defined hollow nanostructure have been rarely reported. Herein, a simple synthetic scheme to prepare Ir-based hollow nanocages of ternary alloy with tunable morphology and size will be reported. The prepared Ir-based hollow nanocages with ternary composition showed excellent electrocatalytic activity and durability toward OER under acidic condition.

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Hole punched Cu3P nano-platelets with controllable plasmonic property

주진환 이광렬*

고려대학교 화학과

Surface plasmons (SPs) are due to surface-bound delocalized electron oscillations formed at the interface of a plasmonic material and a dielectric medium. These phenomena are very sensitive to the surface refractive index change and also have a great potential to monitor the binding events in biological/chemical systems. However, most of the SPs researches are focused on novel metals such as gold and silver, which are highly expensive. Herein, we report hole punched copper phosphide as a well-suited plasmonic system for the usage in biological/chemical sensor and optoelectronics. Because of strongly coupled plasmons at inner and outer surfaces, these hole punched structures are particularly attractive for various sensing applications.

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Template-mediated synthesis of metal-doped nanostructure

김태경 이광렬*

고려대학교 화학과

Template-mediated growth of nanoparticles is a very efficient method to synthesize well-defined hollow or hierarchical colloidal nanocrystals. Typically, the template can be used as a platform where other materials are deposited by the reduction of precursor. Furthermore, template components are released out by the dissolution of template itself. On the other hand, dopants (metal ions) can play an important role to construct interesting nanostructures through interaction between other cations and anions during synthesis. Therefore, various types of shape-controlled nanoparticles can be obtained from template-mediated synthesis for versatile applications such as optics, sensors, water splitting, fuel cell, and so on. In this study, we developed a facile synthetic method of hetero-nanostructured particles induced by metal doping of metal sulfides, which might find interesting applications in optics and catalysis.

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Synthesis of Ru-NiP hetero-dimeric nanoparticle and its bi-functional ability toward water splitting

진하늘 이광렬*

고려대학교 화학과

Metal phosphide nanomaterials are known as great electrocatalysts toward photo/electro-chemical hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). Notably, nickel phosphide has received a considerable attention for its great activity and stability in both acidic and alkaline media. Recently, we found that mild reaction conditions lead to the advent of new phosphide nanoparticles in terms of morphology and composition. Herein, we successfully synthesized Ru-NiP nanoparticle with a fused dimeric structure. Interestingly, Ru-NiP exhibits bifunctional electrocatalytic ability toward both HER and OER in acidic media.

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Synthesis of quaternary hetero double layered nanoframe toward oxygen evolution reaction

박종식 이광렬*

고려대학교 화학과

Nanoframes with open architectures hold a great promise for various applications due to their inherent high surface area. In order to increase the catalytic activity and stability toward water splitting, we suggest a structural motif of double layered nanoframe for RuIr based quaternary system, which has been reported to show excellent electrocatalytic performance in oxygen evolution reaction (OER). Herein, we demonstrate a facile one-pot synthesis of quaternary double layered nanoframe by controlling the precursor decomposition steps and accompanying electrocatalytic activity toward oxygen evolution reaction.

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Synthesis of hollow cobalt and nickel sulfide nanocages using sulfidation and cation exchange method

김준 이광렬*

고려대학교 화학과

Since demand for a new class of energy material is expected to rise, developing inexpensive and high-performance materials for energy conversion and storage applications is the matter of concern for both science and industry. While precious metal (Pt, Ir, Ru)-based materials have shown unmatchable performance in various applications, transition metal oxide materials are still struggling to meet the high standards due to their intrinsic nature such as low conductivity and weak structural integrity. However, transition metal sulfide materials, owing to their unique physical and chemical properties, possess interesting yet crucial characteristics such as metallic properties and structural tolerance in acidic media. Herein, we report the synthesis of hollow Co9S8 and Ni9S8 nanocages by from CoO template, which are expected to show excellent electrocatalytic performance toward water splitting.

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Synthesis of Au@CoS nanoparticle and its potential as an electrocatalyst in oxygen evolution reaction

박지솔 김준 이광렬*

고려대학교 화학과

While hydrogen is considered one of the most promising energy sources in the future, the production of hydrogen is heavily dependent on fossil fuel processing. Environment-friendly method such as water electrolysis requires highly efficient yet expensive electrocatalysts such as Pt, IrO2 and RuO2. Therefore, developing cost-effective catalysts based on earth-abundant metals is on demand. In this regard, metal sulfide exhibits crucial characteristics including metallic properties and structural tolerance in acidic media, which are favorable toward water splitting reaction. In this work, we report the synthesis of Au@CoS core-shell nanoparticle and its potential to be used as an electrocatalyst in oxygen evolution reaction.

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Highly active Au@Pt3Ni nanowire electrocatalysts toward oxygen reduction reaction

양유진 권태현 진하늘 이광렬*

고려대학교 화학과

Platinum-nickel alloys have received great attention due to their optimal surface electronic structure in oxygen reduction reaction. In addition, the optimization of d-band center of Pt alloys is critical issue to enhance the electrocatalytic performance of ORR. Also applying lattice strain of Pt atoms has been found to be important in enhancing catalytic activity. Herein, we synthesized Au@Pt3Ni nanowires with a core-shell bead structure, which possesses both tensile strain at the core and compressive strain at the surface. We expect this synthetic material could greatly widen avenues to enhanced performances toward oxygen reduction reaction.

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장소: 일산 KINTEX

발표코드: **INOR.P-137**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Metal-doped Ir based trimetallic nanocages as electrocatalytically active and stable catalysts toward oxygen evolution reaction

최송아 박종식 이광렬*

고려대학교 화학과

Iridium based nanoparticles are most widely used electrocatalysts for oxygen evolution reaction (OER) due to their high activity and durability, but use of the noble metals has limitation in industrial usage because of its high price. Therefore, we synthesized transition metal–doped IrNi alloy to reduce the amount of Ir and fabricate a cost-effective electrocatalyst. Herein, we report synthesis of transition metal-doped IrNi hollow nanostructures and their high performances toward oxygen evolution reaction.

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Carbon dioxide adsorption in heterodiamine-functiomalized M_2(dobpdc) frameworks

김정은 송정화 강동원 이한글 이화영 강민정 엄선휘 홍창섭*

고려대학교 화학과

A series of metal-organic frameworks M_2(dobpdc) (M = Mg, Mn, Co, Ni, Zn ; H_4(dobpdc) = 4,4'-dihydroxy-1,1'-biphenyl-3,3'-dicarboxylic acid) was synthesized by microwave or solvothermal reactions. N,N-dimethylethylenediamine (dmen) is heterodiamine, which has primary and tertiary amine. Using post modification method, dmen-functionalized M_2(dobpdc) was prepared. It has high selectivity for CO_2 adsorption over N_2 and high working capacity. The structure was characterized via X-ray diffraction, infrared spectroscopy and thermogravimetric analysis. In this study, we focused on sorption properties of dmen-functionalized M_2(dobpdc) and compared CO_2 adsorption capacities.

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Carbon dioxide adsorption capacity in expanded MOF-74 series functionalized with amines

주은경 이화영 홍창섭*

고려대학교 화학과

We functionalized Mg_2(dobpdc) with a series of linear aliphatic diamines of ethylenediamine, 1,3-diaminopropane, 1,4-diaminobutane, hexamethylenediamine, and 1,8-diaminooctane. The structure was verified via X-ray diffraction and 1H NMR. The solids were characterized via infrared spectroscopy, thermogravimetric analysis, and sorption. Detailed synthetic scheme and specific properties will be presented in the poster.

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Monoamine-modified Mg_2(dobpdc) with different chain lengtsh and their characterizations

엄선휘 송정화 강동원 이한글 이화영 김정은 강민정 홍창섭*

고려대학교 화학과

We functionalized Mg_2(dobpdc) with various kinds of linear aliphatic monoamines.: methylamine, ethylamine, propylamine, butylamine, pentyllamine, and hexylamine. These structures were identified with X-ray diffraction via Pawley refinement. Also, they were characterized via thermogravimetric analysis, infrared spectroscopy, and sorption. Detailed synthetic scheme and specific properties will be presented in the poster.

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Synthesis, characterizations, and magnetic studies in two-dimensional lanthanide complexes

송정화 강동원 이한글 홍창섭*

고려대학교 화학과

We have synthesized four isostructural two-dimensional flexible coordination polymers, $[Ln(p\text{-}XBP4)_{2.5}(H_2O)_3(CH_3OH)_3]\bullet W(CN)_8\bullet nCH_3OH$ (Ln=Dy, Tb, Er, Gd) ($p\text{-}XBP_4$=N,N'-*p*-phenylenedimethylenebis(pyridin-4-one)) using a slow evaporation method. Each Ln^{3+} ion is coordinated by five oxygen atoms from $p\text{-}XBP_4$ ligand and two oxygen atoms from water molecules. Tungsten octacyanide exists in the anionic form for charge balance. Compounds were characterized by elemental analysis, IR, PXRD and single crystal X-ray diffraction. Detailed structural and magnetic studies will be given in the presentation.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

A New Hydrogen-bonded Organic Framework and its Characterizations

김지형 강동원 홍창섭*

고려대학교 화학과

We synthesized a new hydrogen-bonded organic framework, 1, from tetrakis(4-sulfophenyl)methane and guanidine hydrochloride via slow evaporation for 5 days. The structure of compound 1 was confirmed by single crystal X-ray diffraction, and its framework was confirmed consisting of hydrogen bonding among reactants and solvents. Additionally, the compound was characterized by powder X-ray diffraction, infrared spectroscopy, thermogravimetric analysis, scanning electron microscope, and sorption. Detailed synthetic scheme and several properties will be given in the presentation.

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Development of a Superprotonic Porous Organic Polymer Conductor via a Postsynthetic Method

강동원 송정화 이한글 김정은 이화영 강민정 엄선휘 홍창섭*

고려대학교 화학과

We synthesized a porous organic polymer compounds, 1, and modified it to 1S via direct post-synthetic substitution using chlorosulfonic acid. Compounds were characterized by infrared spectroscopy, thermogravimetric analysis, X-ray photoelectron spectroscopy, ^{13}C Solid state nuclear magnetic resonance, sorption and impedance spectroscopy. Especially, 1S showed the superprotonic performance (7.72 x 10^{-2} S cm^{-1}) among porous organic materials reported to date. Also, Membrane Electrode Assembly test were executed. Detailed synthetic scheme and several properties will be given in the presentation.

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Shaping Metal-Organic Framework to improve strength and carbon dioxide adsorption

이화영 송정화 강동원 이한글 김정은 강민정 엄선휘 홍창섭*

고려대학교 화학과

We functionalized magnesium MOF with amine. Usuing binder, we synthesized shaping MOF to improve strength. These compounds were characterized by X-ray diffraction via Pawley refinement, infrared spectroscopy, X-ray photoelectron spectroscopy and sorption. Especially, working capacity were evaluated by thermogravimetric analysis (CO_2 15% / N_2 85%). Detailed synthetic scheme and specific properties will be presented in the poster.

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발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Improvement of mechanical strength of MOFs shaped with silica for CO_2 capture

강민정 송정화 강동원 이한글 김정은 이화영 엄선휘 홍창섭*

고려대학교 화학과

We synthesized amine-functionalized Mg-MOFs using silica as a binder. The synthesized MOFs showed improved mechanical strength and showed significant adsorption capacity. These compounds were confirmed by powder X-ray diffraction, infrared spectroscopy and sorption. Additionally, carbon dioxide adsorption capacity were evaluated by thermogravimetric analysis. Detailed synthetic scheme and specific properties will be presented in the poster.

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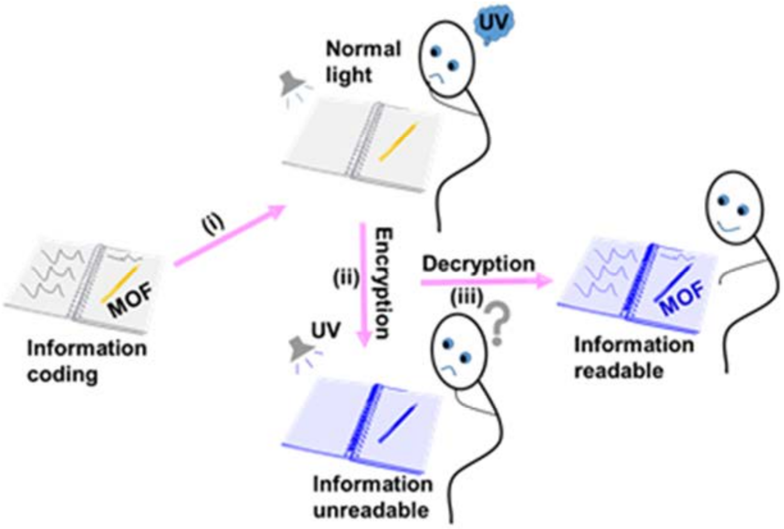
Easily Transferable Metal-Organic Framework Security Ink

김의수 윤민영[1,*] 박경세[2,*]

가천대학교 글로벌캠퍼스 화학과 [1]가천대학교 글로벌캠퍼스 나노화학과 [2]군산대학교 화학과

To date, ample of materials such as quantum dots, dyes etc., have been widely applied as security ink to secrecy the data information and detection of toxic metals. Nevertheless, due to the poor dispersibility of solid state materials, security ink based on a solid state material has been scarcely reported. In this concern, highly dispersible and water stable metal-organic framework (NH2-MIL 125) can be a candidate for the application due to its strong photoluminescent for data coding, encryption and decryption by invisible security ink. Its distinguishing properties such as uniform nanosize, high quantum yield, large surface area, and high stability in air and water allows facile application as a security ink. The strong photoluminesce was quenched by the addition of Pb2+ ions, which was recovered upon addition of EDTA solution for the removal of Pb2+ ions. In addition, the MOF solution was easily transferred by writing and stamping on a paper and demonstrates encryption and decryption behavior for security ink application. The details of the mechanism study for photoluminesce turn on and off will be presented.


Normal
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(iii)
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Information
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UV
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MOF
Information
readable

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-147**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Temperature dependent CO_2 behavior in microporous 1-D channels of a metal-organic framework

김동욱 한승완 나명수*

UNIST 화학과

The observation of encapsulated carbon dioxide (CO_2) molecule is one of the important issues to understanding about those activation environment for utilization of CO_2 molecules. Metal-organic frameworks (MOF) are crystalline and porous materials, thus some of MOF structures could be applied to container or cage for gas capture and separation. Here we synthesized new Cu-MOF, $[Cu_3Cl_2(\text{tetrazole})_4]$, which has microporous 1-D channels structure with neck-like portal window of ~2.5 Å in diameter. The encapsulated CO_2 molecules in this MOF structure with pressurized CO_2 are analyzed by single crystal X-ray diffraction (SCXRD). The CO_2@Cu-MOF were showed different multiple interaction between MOF structures and CO_2 molecules depended on temperature. In this presentation, we will discuss observed structures and temperature dependent CO_2 uptakes as gas sorption experiment.

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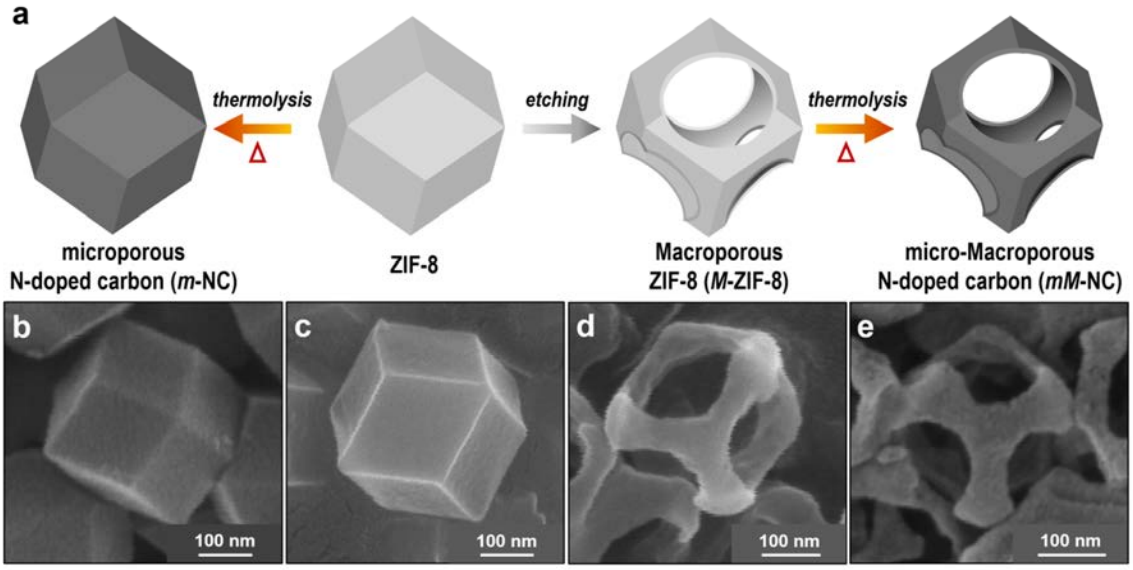
New synthetic approach for macorporous N-doped cabon materials via thermolysis of ZIF-8

주인태 정성은[1] 문회리[2,*]

UNIST 분자과학부 [1]UNIST 친환경에너지공학부 [2]UNIST 화학과

In order to achieve the advantage of macroporosity in porous carbon materials such as large surface area and mass transport and diffusion, a lot of efforts have been made. So far, macro- and mesoporous carbon materials have been synthesized by using sacrificial templates such as mesoporous silica, and polymer beads. Recently, metal-organic frameworks (MOFs) receive a spotlight as a precursor towards porous carbon materials since it can establish the template-free system for synthesizing nanoporous carbon via thermal conversion. We recently reported the synthesis of micro- and meso-porosity tuned nanoporous carbon by employing the Zn-MOF as a precursor by controlling thermolysis conditions. Herein, we report a template-free synthesis of micro-macroporous carbon. By using wet-chemical etching of rhombic dodecahedron ZIF-8 crystals, we produce macroporous ZIF-8 with four openings and walls, which is attributed to the surface-selective reactivity. Through the pseudomorphic conversion, macroporous ZIF-8 can be converted to macropore-tuned nitrogen-doped carbons (100 ~ 200 nm). In lithium air battery as one of the most prominent battery systems, there has been a critical issue on introducing the air electrode that enables the mass transport and rapid diffusion of oxygen and sustains the precipitation of the discharged products of Li2O2. We demonstrate the utility of the macroporous carbon in enabling the accessibility of the oxygen and preventing the discharged products from blocking in the air electrode.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thermolysis
Δ
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thermolysis
Δ
microporous
N-doped carbon (*m*-NC)
ZIF-8
Macroporous
ZIF-8 (*M*-ZIF-8)
micro-Macroporous
N-doped carbon (*mM*-NC)
b
100 nm
c
100 nm
d
100 nm
e
100 nm

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Reactivity of a Cobalt(III)-Hydroperoxo Complex in Electrophilic Reactions

신봉기 조재홍*

DGIST 신물질과학

The reactivity of mononuclear metal–hydroperoxo adducts has fascinated researchers in many areas due to their diverse biological and catalytic processes. In this study, a mononuclear cobalt(III)–peroxo complex bearing a tetradentate macrocyclic ligand, $[Co^{III}(Me_3\text{-TPADP})(O_2)]^+$ (Me_3-TPADP = 3,6,9-trimethyl-3,6,9-triaza-1(2,6)-pyridinacyclodecaphane), was prepared by reacting $[Co^{II}(Me_3\text{-TPADP})(CH_3CN)_2]^{2+}$ with H_2O_2 in the presence of triethylamine. Upon protonation, the cobalt(III)–peroxo intermediate was converted into a cobalt(III)–hydroperoxo complex, $[Co^{III}(Me_3\text{-TPADP})(O_2H)(CH_3CN)]^{2+}$. The mononuclear cobalt(III)–peroxo and −hydroperoxo intermediates were characterized by a variety of physicochemical methods. Reactivity studies performed with the cobalt(III)–peroxo and −hydroperoxo complexes in organic functionalizations reveal that the latter is capable of conducting oxygen atom transfer with an electrophilic character, whereas the former exhibits no oxygen atom transfer reactivity under the same reaction conditions. Alternatively, the cobalt(III)–hydroperoxo complex does not perform hydrogen atom transfer reactions, while analogous low-spin Fe(III)–hydroperoxo complexes are capable of this reactivity. Density functional theory calculations indicate that this lack of reactivity is due to the high free energy cost of O–O bond homolysis that would be required to produce the hypothetical Co(IV)–oxo product.

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발표분야: 무기화학
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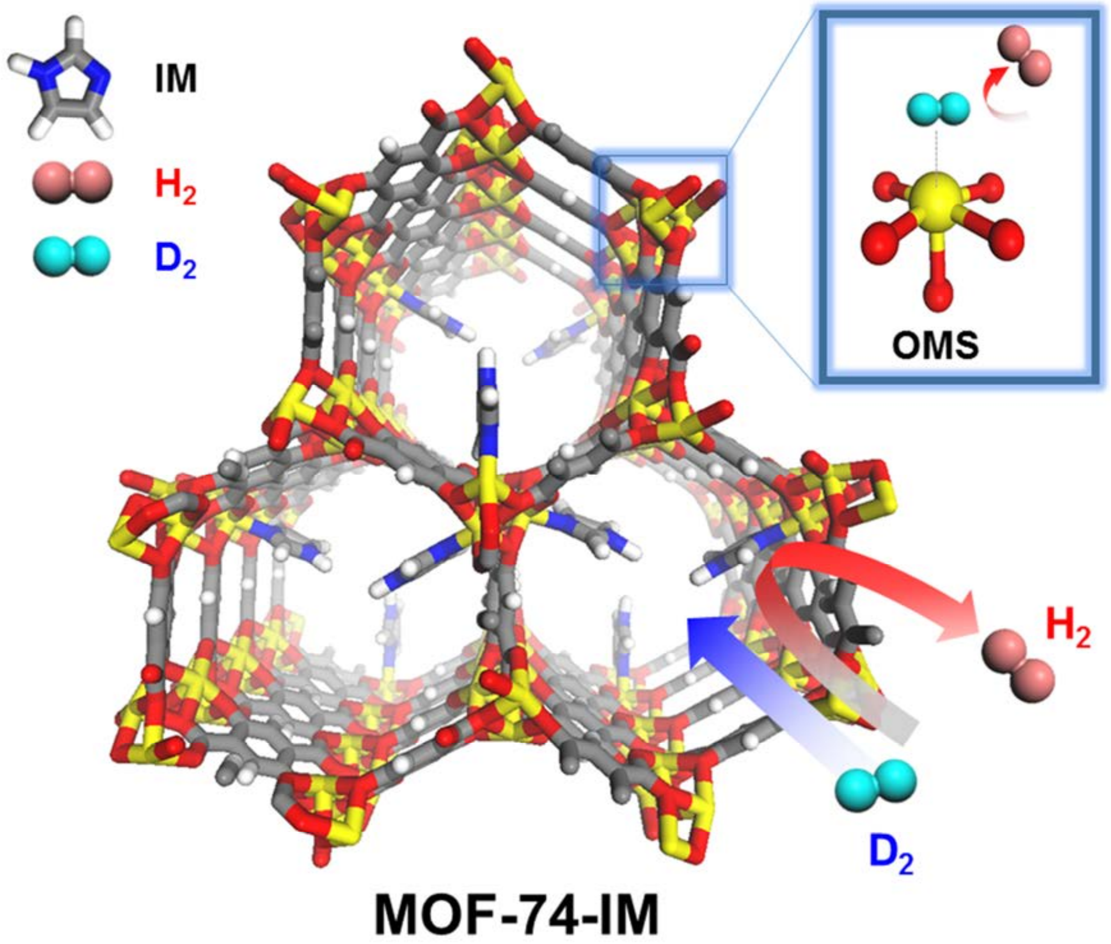
Synergy of Open Metal Sites and Diffusion Barrier in a Metal-Organic Framework for Highly Effective Hydrogen Isotope Separation

김진영 문회리*

UNIST 화학과

The increasing demands of D_2 in neutron scattering techniques, isotopic tracing, and fission reactors as a cold source accelerate the separation technology for D_2. The current separation technologies for the heavy hydrogen isotopes are extremely energy intensive, and low separation efficiency leading to the major issues in the nuclear industry. For example, conventional hydrogen isotope separation techniques, such as liquid hydrogen distillation and girdler sulfide process, are highly energy- and time- intensive; nonetheless, they provide only low separation factor (i.e. cryogenic distillation, selectivity of 1.5 at 24 K), which stimulates the exploration of the alternative separation system.Herein, we report a highly effective hydrogen isotope separation system based on metal-organic frameworks (MOFs) having a separation factor as high as ca. 26 at 77 K by maximizing synergistic effects of chemical affinity quantum sieving (CAQS) and kinetic quantum sieving (KQS). To the best of our knowledge, this is the first attempt combining the KQS and CAQS effects to separate D_2 in hydrogen isotope mixture.


IM
H_2
D_2
OMS
H_2
D_2
MOF-74-IM

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장소: 일산 KINTEX
발표코드: **INOR.P-151**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Topology conversions of non-interpenetrated metal-organic frameworks to doubly interpenetrated metal-organic frameworks

정석 임재웅 나명수*

UNIST 화학과

Non-interpenetrated 3D metal-organic frameworks (MOFs) with both an interpenetration-favorable (3,5)-c hms topology and an interpenetration-unfavorable (3,5)-c gra topology are converted to doubly interpenetrated analogues with hms-c topology by thermal treatment, even in the absence of solvent. Depending on conversion temperature and the properties of the pillaring ligand in the non-interpenetrated 3D MOF, which is based on 2D sheets with 3-c hcb topology pillared by neutral ditopic linkers, the pillaring ligands in the interpenetrated MOFs produced are partially removed during the thermal conversions, leading to interpenetrated MOFs that simultaneously contain both micro- and mesopores.

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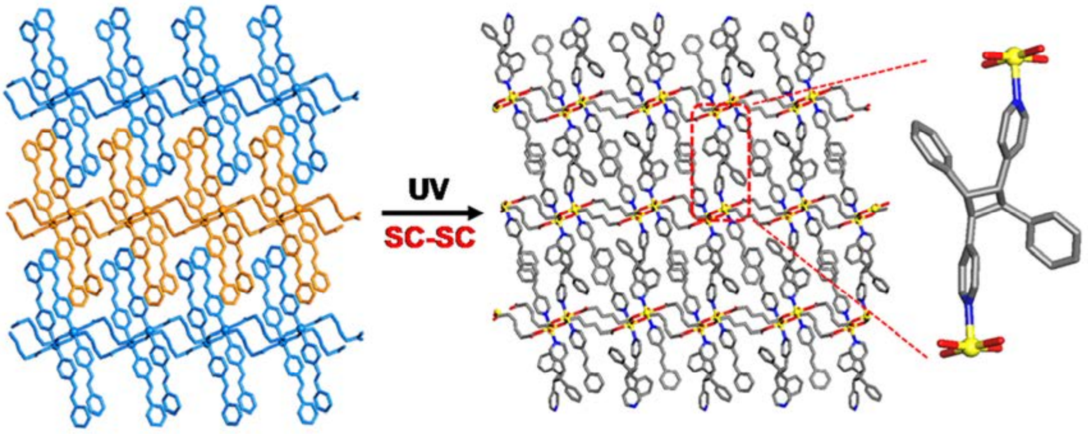
Single-crystal-to-single-crystal transformation of a coordination polymer from 2D to 3D by [2 + 2] photodimerization assisted by a coexisting flexible ligand

이재화 정성은[1] 문회리[*]

UNIST 화학과 [1]UNIST 친환경에너지공학부

A 2D interdigitated [$Ni_2(adipate)_2(spy)_4(H_2O)_2$] (spy = 4-styrylpyridine) was transformed to a 3D coordination polymer through [2 + 2] photodimerization between the olefin bonds in spy upon UV-irradiation in a single-crystal-to-single-crystal (SC–SC) manner. During this transformation, a coexisting flexible adipate ligand changes its conformation, and helps in withstanding the conversion strain and retaining the single crystallinity.



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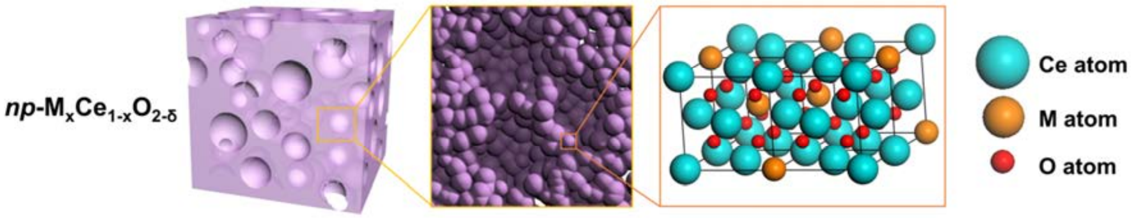
Facile Synthesis and Characterization of Nanostructured Transition Metal-Ceria Solid Solutions ($TM_xCe_{1-x}O_{2-\delta}$, TM = Mn, Ni, Co, Fe) for CO Oxidation

이경주 이재화 문회리*

UNIST 화학과

We developed a general synthetic route to prepare nanoporous transition metal-ceria solid solutions with nanocrystalline frameworks ($TM_xCe_{1-x}O_{2-\delta}$, TM = Mn, Ni, Co, and Fe). Their structural properties were characterized by using transmission electron microscopy (TEM), X-ray powder diffraction (XRPD), and N_2 sorption. Through thermolysis of bimetallic coordination polymers, hierarchically nanoporous frameworks composed of 3 - 4 nm-sized $TM_xCe_{1-x}O_{2-\delta}$ solid solution nanocrystals were synthesized, in which the transition metal ions are well-dispersed in the ceria lattice as evidenced by the Rietveld refinement of the XRPD patterns. The electronic properties of the $Mn_xCe_{1-x}O_{2-\delta}$ solid solutions with up to 20 mol% were examined by Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS) analysis, and H_2-temperature-programmed reduction (TPR) results demonstrated the altered physicochemical properties, e.g. hydrogen reduction behaviors, due to the doping. CO-oxidation studies of $Mn_xCe_{1-x}O_{2-\delta}$ reveal that the Mn species are responsible for increasing the catalytic activity by an order of magnitude compared to pure ceria, by creating nanostructures with accessible pores and active sites on the inner surface. This facile synthetic approach can create nanoporous solid solutions with nanocrystalline frameworks and devise structures and compositions. Therefore, it opens new avenues for developing multi-metallic catalyst systems.



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Synthesis and promising applications of nano-cup shaped silica nanoparticles stabilized in aqueous nano colloids at ambient temperature

김선옥 이인수[1,*]

포항공과대학교 화학과 [1]POSTECH 화학과

Up to date, diverse nano-cup shaped particles made of silica or metals have been reported for various potential applications such as catalyst, energy storage device, biosensor, drug delivery and so on. Although cup-shaped particles have been reported, the synthesis of nano-scale particles are limited in hundreds of nanometers. In this work, cup-shaped nanoparticles are newly synthesized in 35-40nm diameter scale using Janus nanoparticles of Fe_3O_4 encapsulated in amino-silane in water solution at room temperature. Each initially spherical nanoparticle creates a cavity leading to final cup-shape. The designed cup-shaped nanoparticles are stable in aqueous solution over 1 month. Because of unique physiochemical properties, we anticipate that this cup-shaped nanoparticle has a great possibility to be used in broad biomedical and healthcare product applications.

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Indium-salen Complexes as a Novel Class of Luminophores

곽상우 우원희[*] 현경림[*] 김영조[*] 이강문[1,*] 박명환[2,*]

충북대학교 화학과 [1]강원대학교 화학과 [2]충북대학교 화학교육과

Organometallic complexes based on group 13 metals such as aluminum and gallium have been recently reported as optoelectronic materials due to thier intriguing electronic and photophysical properties. The aluminum salen complexes have widely been investigated as outstanding luminophores in diverse optoelectronic materials due to their intriguing photophysical properties. Along with these studies, several heterodinuclear systems based on Al-salen compounds have recently been reported.[1] In this regard, we explore a novel class of color-tunable luminophores, we investigated salen based indium complexes, which are heavier congener systems of well-known liminoscent Al-salen complexes. There have been no reported studies on monomeric indium complexes that display multicolor emission features due to the simple alteration of thier substituents. In a continuous effort to we have prepared a series of salen based indium complexes and investigated the emissions induced by these complexes in detail. The detailed synthesis, characterization, and photophysical properties of the dyads were described.

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Transformation of $MnO@SiO_2$ Core@Shell Structured Nanosphere Toward a Highly Porous Mn_3O_4 Nanoparticle Embedded in SiO_2 via Nanospace Confined Solid State Reaction

권태완 이인수[1,*]

포항공과대학교 화학과 [1]POSTECH 화학과

Preparation of the highly porous materials has been extensively performed due to various advantages such as large surface area, controlling pore size, flexible frameworks, etc. Generally, porous Mn_3O_4 particles (p-Mn_3O_4) have been synthesized by using sacrificial templates through solution process, which is restricted to convert into a new composition due to limited available precursor in a certain solvent and chemical reaction. However, chemical conversion into a new composition can be widely expanded via solid-state reaction because of almost unlimited available elements. To best of our knowledge, there is no report to prepare p-Mn_3O_4 particles due to sintering during high temperature reaction. Herein, we report for the first time to prepare p-Mn_3O_4 nanoparticles through nanospace confined solid-state conversion reaction and to provide a mechanistic insight of the transformation from MnO to p-Mn_3O_4.

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Ultra-Thin Layered Carbon Shell Induced Metal-Metal Oxide-Carbon Triple Junction of Mn_3O_4/Pt@C Nanoparticles to Enhance the Electro-catalytic Mass Activity in ORR *via* Fast Dopamine Polymerization on the Surface of Mn_3O_4

이동규 이인수*

POSTECH 화학과

To enhance the electro-catalytic mass activity of fine Pt nanoparticles deposited on Mn_3O_4 nanoparticles while maintaining operational durability and specific activity for oxygen reduction reaction (ORR), we have conducted to alter the thickness of the carbon shell to generate triple-junction of Mn_3O_4-Pt-carbon, producing Mn_3O_4/Pt@C nanoparticles. Herein, we report for the first time that ultra-thin-layered carbon shell encapsulating Mn_3O_4 nanoparticle anchoring high density of Pt nanocatalysts, which showed significantly enhanced mass activity of Pt for ORR with maintaining excellent specific activity and operational durability. It is also worth noting that Mn_3O_4 nanoparticles play a crucial role of fast oxidizing and polymerizing dopamine monomer to form PDA shell, which allows us to prepare ultra-thin PDA shell surrounding Mn_3O_4 nanoparticles. After carbonization process and galvanic replacement reaction with Pt, the Mn_3O_4/Pt@C nanoparticles were obtained. The ultra-thin-layered carbon shell have crucial role for ORR, which admits the diffusion of reactant freely during ORR as well as improves electrical conductivity Mn_3O_4 support.

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발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Direct In situ Conversion of Metals into Metal-Organic Frameworks: A Strategy for the Rapid Growth of MOF Films on Metal Substrates

지훈 황선현[1] 정낙천[2,*]

DGIST 신물질과학전공 [1]DGIST 신물질과학 [2]DGIST 신물질과학과

The fabrication of metal−organic framework (MOF) films on conducting substrates has demonstrated great potential in applications such as electronic conduction and sensing. For these applications, direct contact of the film to the conducting substrate without a self-assembled monolayer (SAM) is a desired step that must be achieved prior to the use of MOF films. In this report, we propose an in situ strategy for the rapid one-step conversion of Cu metal into HKUST-1 films on conducting Cu substrates. The Cu substrate acts both as a conducting substrate and a source of Cu2+ ions during the synthesis of HKUST-1. This synthesis is possible because of the simultaneous reaction of an oxidizing agent and a deprotonating agent, in which the former agent dissolves the metal substrate to form Cu2+ ions while the latter agent deprotonates the ligand. Using this strategy, the HKUST-1 film could not only be rapidly synthesized within 5 min but also be directly attached to the Cu substrate. Based on microscopic studies, we propose a plausible mechanism for the growth reaction. Furthermore, we show the versatility of this in situ conversion methodology, applying it to ZIF-8, which comprises Zn2+ ions and imidazole-based ligands. Using an I2-filled HKUST-1 film, we further demonstrate that the direct contact of the MOF film to the conducting substrate makes the material more suitable for use as a sensor or electronic conductor.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **INOR.P-159**

발표분야: 무기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Transformation of Pt-Fe_3O4_4 Nanoparticle Encapsulated within a Hollow Silica into FePt/Fe Heterodimer Structure Induced by FePt Migration Toward SiO_2

박수현 이인수[1,*]

포항공과대학교 화학과 [1]POSTECH 화학과

The solid state conversion chemistry of nanoparticles in the SiO_2 media by annealing was attractive subject, which can provide the observation of the interaction between two different phase materials with detailed information due to confinement of the precursors within a tens-of-nanometer. To systematic study the interaction at the interface of the metal and SiO_2 during annealing process, Pt deposited on the surface of Fe_3O4_4 nanoparticles encapsulated by SiO_2 after annealing process, generating yolk-shell type structure. After the reductive annealing (4% H_2, 96% Ar), dumbbell-like FePt/Fe heterodimer formed in the cavity of the SiO_2. During this process, we observed that structure transformation from core@shell structure of FePt@Fe to heterodimer structure of FePt/Fe occurred in the hollow SiO_2 shell. Surprisingly, the FePt core migrated toward the interface of SiO_2 and Fe during the transformation. This interesting phenomena observed could be ascribed to the high interfacial energy between FePt and Fe, which was the driving force of the phase transformation. Our new finding can give an important insight for studying metal migration on the support in harsh catalytic reaction condition.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Progressive Report on the Development of Resonance Laser-Assisted Sputtered Neutral Mass Spectrometer for Uranium Isotope Analysis in the Presence of Isobaric Elements

박진규* 임상호 이치규 한선호[1]

한국원자력연구원 원자력화학연구부 [1]한국원자력연구원 분석화학실

Today, mass spectrometric techniques contribute enormously to the fields of nuclear safeguards and nuclear forensics, providing crucial information to examine undeclared nuclear activity. Among others, resonance laser-assisted sputtered neutral mass spectrometry (RL-SNMS) is a rare and developing method, which is able to selectively analyze an atom of interest in the presence of isobaric elements. For example, ^{238}U interferes with ^{238}Pu and ^{241}Pu does with ^{241}Am. Each pair requires extremely high mass resolving power (m/dm > 105) to be analyzed by conventional mass spectrometric tools.In this study, 3-color Ti:Sapphire laser with wavelength tunability was combined with time-of-flight mass spectrometer (TOF-MS) installed with gallium liquid metal ion gun, in order to build a RL-SNMS system. Gadolinium (Gd) plate and U solution dried on a silicon wafer were prepared for the experiment, because Gd needs a similar excitation wavelength scheme to Pu. In order for the resonance excitation of Gd or U to occur in the sample chamber of TOF-MS, 3-color laser beams were collinearly aligned, and the beam pulses were matched within several dozen of nanoseconds. The wavelengths were tuned with the previously reported ones specific for the excitation of uranium, and confirmed by a wavemeter. Timings of primary ion beam pulse, laser beam pulses and stage voltage pulse on TOF-MS were synchronized for the detection of laser-ionized ions. The progress so far will be discussed in the poster presentation.

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Synthesis of Thiourea Functionalized Metal-organic Cage

김현용 이은성*

POSTECH 화학과

Metal-organic cages consisting of metal ions and organic linkers have well defined structures and moderate solubility in various organic solvents. The properties of the metal-organic cages are expected to be easily tuned by modification of organic ligand and metal ion. The cage compounds have been utilized in the various fields such as separation, catalysis. Due to the easy tunability, metal-organic cage having thiourea can be prepared by using the appropriate organic linker having thiourea moieties. Here, we report a discrete metal-organic cage having thiourea moieties by the reaction of 1,3-bis(2,6-diisopropyl-4-((E)-(pyridin-2-ylmethylene)amino)phenyl)-1H-imidazole-2(3H)-thione with Zinc di[bis(trifluoromethylsulfonyl)imide]. The resulting cage which was characterized by NMR as well as ESI-MS may be applicable to the selective detection and removal of highly toxic mercury ion.

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장소: 일산 KINTEX
발표코드: **INOR.P-162**
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Nickel(Ⅱ) and Cobalt(Ⅱ) Coordination Polymer from a Metallascorpionate Ligand

이슬기 이준승[*]

전남대학교 화학과

There have been much attentions to hetermetallic coordination compounds due to their interesting electronic and physical properties. Previously we reported Fe-M hetereometallic complexes (IPtz) possessing three 5-(2-hydroxyphenyl)tetrazole. IPtz had two different binding site (nitrogen triangle site and oxygen triangle site and two different sites were used in the complexation with different metal centers. As a result, we successfully synthesized Zn-Fe-K heterometallic coordination polymer. In this study, we extended the system to other transition metal ions including Co^{2+} and Ni^{2+}. Nickel(Ⅱ) and Cobalt(Ⅱ) coordination polymer were synthesized by the simple assembly of IPtz and K, Ni/Co precursors, and structures of the complexes were determined by X-ray diffraction studies. The extended structures of complex showed honeycomb shape and had vacant holes that would be good for selective gas absorption.

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장소: 일산 KINTEX
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Bimetallic Supramolecules with Tripodal Homo- or Heteroleptic Metalloligands

이지민 이슬기 이준승*

전남대학교 화학과

In the supramolecular chemistry, precious structural modulation of supramolecule is one of interesting research subjects. *β*-diketonate ligands with pyridyl group, acting as a chelating ligand to the primary metal center, were prepared and used in the self-assembly. They have additional binding sites provided by pyridyl groups and can be involved in the self-assembly to construct highly complicated supramolecules. We designed and synthesized several metalloligands possessing with trichelate Al^{3+} octahedral center and *β*-diketonate ligand like *tris-{1-(4-pyridyl)acetylacetonato}* or *mono-, bis- {1,3-di(4-pyridyl)-1,3-propanedionato}*. Self-assembly of *(tris-{1-(4-pyridyl)acetylacetonato})Al(Ⅲ)* and diruthenium electron accepters resulted in the formation of [2 + 3] heterometallic coordination cage. And *(di(4-pyridyl)-1,3-propanedionato)*$_2$*(acetylacetonato)Al(Ⅲ)* and 90° platinum acceptor was reacted to produce [2 + 4] heterometallic rectangular supramolecule.

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Chemical environment control of molecular photocatalyst within MOF

류언진 최경민[1,*]

숙명여자대학교 화공생명공학과 [1]숙명여자대학교 화공생명공학부

Molecular catalysts are typically used as a discrete unit having free-motion in solvents, so it has been challenging to design the spacial condition that the catalytic reactions are taking place. In this report, we demonstrated how the molecular catalysts can be designed on their environment chemically controlled by using the facility with which metal-organic frameworks (MOFs) can be functionalized, and show a fine balance of proximity in between functional groups and molecular catalysts enhances the photocatalytic activity for carbon dioxide conversion under visible light by their cooperatively enhanced reaction mechanism. Specifically, we choose a functional group of amine ($-NH_2$) as chemical functionality, incorporated into Re-MOF that $ReI(CO)_3(BPYDC)(Cl)$, BPYDC = 2,2’-bipyridine-5,5’–dicarboxylate, is covalently attached within a zirconium-based MOF, and controlled the amount of $-NH_2$ group to the total amount of organic linkers. We found that the $-NH_2$ functional group contributes to the enhanced photocatalytic activity by making the molecular structure of Re complex asymmetric and the CO_2 intermediate within Re-MOF-NH_2(33%)

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **INOR.P-165**
발표분야: 무기화학
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Ruthenium nitrosyls complex with Bis(diamino-diamido)tetrathiafulvalene (BDD-TTF)

조장훈 <u>KhanMohammadSherjeelJaved</u> 이홍인*

경북대학교 화학과

The coordination chemistry of tetrathiafulvalene(TTF) derivatives has focused a lot of attention towards the development of electroactive transition metal complexes with original electronic properties due to interplay between the TTF and the electron density on the metal. To study these interactions between the TTF moiety and the metal center, another approach has been recently developed which relies on bioinorganic chemistry. Here we have designed a new π-extended analogue of tetrathiafulvalene (TTF), namely, the bis(diamino-diamido)-tetrathiafulvalene(BDD-TTF) and ruthenium nitrosyls compound. Thus, in our work, the present studies explore a different synthetic platform to prepare photoactive ruthenium nitrosyls, the bis(diamino-diamido)-tetrathiafulvalene ligand containing to be tested as a model NO-releasing agent. It has been characterized by various analytical methods.

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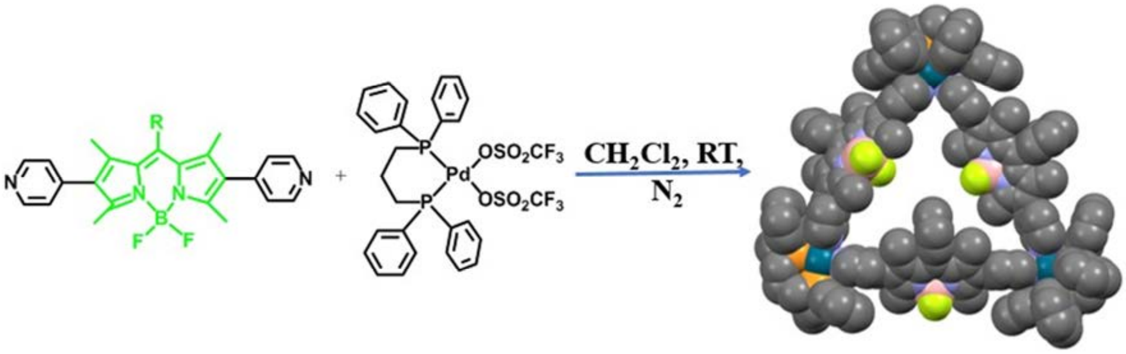
Self-assembled Novel BODIPY-based Pd Supramolecules

GUPTA GAJENDRA 박경철[1] 이선웅[1] 이창연*

인천대학교 에너지 화학공학과 [1]인천대학교 에너지화학공학과

Novel Pd metal supramolecules with triangular/square architectures derived from boron-dipyrromethane (BODIPY) ligands were synthesized by self-assembly and fully characterized by 1H NMR, 31P NMR, ESI-MS and a single crystal XRD. The existence of these supramolecules are solvent dependent and exhibited an equilibrium between the triangular and square molecular architectures in low-polarity solvents, and an increase in solvent polarity shifted these equilibrium towards the triangular architectures.1 These supramolecules were more cytotoxic to brain cancer cells than to normal lung fibroblasts and were found to be more active than the benchmark metal-based drug, cisplatin. The supramolecules also interact strongly with the BSA protein, as well as with Salmon sperm DNA. The characteristic green fluorescence of the BODIPY ligand in these supramolecules permits intracellular visualization of complexes using confocal microscopy, and detects the localization of the compounds in the cytoplasm and on the plasma membrane.2References:1. Cook, T. R.; Stang, P. J. Chem. Rev. 2015, 115, 7001-70452. Gupta, G.; Das, A.; Ghate, N. B.; Kim, T.; Ryu, J. Y.; Lee, J.; Mandal, N.; Lee, C. Y. Chem. Comm. 2016, 52, 4274-4277.acknowledgement : 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)


R
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OSO2CF3
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N2

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발표코드: **INOR.P-167**
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발표종류: 포스터, 발표일시: 금 13:00~14:30

BODIPY incorporated Zr-MOFs for a colorimetric sensing of Hg^+

오정석 정유일 박정원 이창연[1,*]

인천대학교 에너지화학공학과 [1]인천대학교 에너지 화학공학과

Metal-organic frameworks (MOFs), consisting of organic building block and inorganic secondary building unit (SBU), have emerged as a promising alternative to conventional porous materials because of their ultra-high surface area, controllable pore sizes, structural diversity 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. Zirconium based MOFs are well known to have high stability because of their strong Zr(Ⅳ)-O bonds in the metal nodes. A new functionalization technique, solvent assisted ligand incorporation (SALI), was developed to efficiently incorporate carboxylate-based functionalities in the Zr-based metal−organic framework, NU-1000. Herein, NU-1000 was functionalized with BODIPY (Boron-dipyrrolmethane) by using SALI approach and it was used for mercury detection.acknowledgment : This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2016R1A2B4010376)

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장소: 일산 KINTEX
발표코드: **INOR.P-168**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis, structure and luminescence properties of silver(I) complexes with organic ligand including four pyridine group

신종원* 문도현[1,*]

한국과학기술정보연구원 대구경북지원 [1]포항가속기연구소 빔라인운영부 생명화학구조팀

Novel supramolecular solids whose topologies depend on the counteranions, $[Ag(pdba)](NO_3)\bullet CH_3OH$ (**1**) and $[Ag(pdba)](CF_3COO)\bullet CH_3OH$ (**2**), have been prepared by the self-assembly of AgX (X = NO_3^-, CF_3COO^-) with *N,N,N´,N´*-tetra-4-pyridyl-benzeneamine (pdba). Complex **1** displays three-dimensional brick-like coordination polymer due to the geometry of silver(I) ions connected with four pyridines of pdba ligand, while complex **2** shows two-dimensional framework structure with honeycomb motif along the ac plane. **1** exhibits a strong visible light emission ranging from violet to red wavelengths, whereas **2** appears a strong violet emission at around 390 nm and a weak visible emission at around 490 nm. In this poster, the detailed preparation of pdba ligand and compounds, crystal structure and luminescence properties will be described.

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발표코드: **INOR.P-169**
발표분야: 무기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Selective Propylene Carbonate Production form CO2 and Propylene Oxide by a Iron Catalyst

이다영

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 CO2 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 CO2 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. An iron complex, {(NO3)Fe(THF)}2 was synthesized and well characterized by various spectroscopic techniques and X-ray crystallography. Solid-state structure reveals the dimeric nature of {(NO3)Fe(THF)}2 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 {(NO3)Fe(THF)}2, reaction conditions were optimized with several variables including pressure, temperature and co-catalyst/catalyst ratio. Under the optimized conditions, {(NO3)Fe(THF)}2 showed unusual catalytic efficiency with propylene oxide. Moreover, our structural analysis of computed intermediates and transition states shows the preorganized geometry of 4- or 5-coordinated Fe-complexes with our NO3 ligand, resulting in stabilization of the octahedral transition states. Further investigation is currently in progress in order to reveal catalyst geometry-activity connection. Detailed catalytic cycle and characterization will be presented.

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장소: 일산 KINTEX
발표코드: **PHYS.P-13**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effects of Sample Container Shape on Agglomeration of Magnetite Nanoparticles by Magnetic Field

진대성 김학진[1,*]

대전과학고등학교 화학과 [1]충남대학교 화학과

Agglomeration dynamics of magnetite nanoparticles under magnetic field are investigated by measuring the change of magnetic weight in different sample containers, cuvette and conical tube. The magnetic weight of the sample increases as the magnetite nanoparticles agglomerate by magnetic field. Analysis of the dynamic change of magnetic weight shows stretched exponential behaviors. Dynamics is slower in the conical tube sample than in the cuvette sample. Difference dynamics in different container is attributed to weaker magnetic field to the sample and potential energy steepening in the conical tube. Some kinetic characteristics involved in the agglomeration such as the distribution function of the rate constant and energy barrier are discussed in details.

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장소: 일산 KINTEX
발표코드: **PHYS.P-14**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cu_2O/CuO Composites Designed for Wastewater Treatment

최다연 장두전*

서울대학교 화학부

Contamination of water is predicted to become a major threat to the ecosystem. To purify the wastewater, many researchers have paid attention to develop catalysts having efficient performances with unique structures. One effective way is to fabricate well-designed structure. Especially 3-D structures with well-designed structures have been extensively explored to enhance their catalytic performances. Here, diverse morphologies of CuO/Cu_2O composites having good catalytic properties for the reduction of 4-nitrophenol in the presence of $NaBH_4$ have been controlled facilely by adjusting the concentrations of NaOH during the wet etching of Cu_2O cubes. The catalytic activity of CuO/Cu_2O composites is found to depend highly on their morphologies; in particular, CuO/Cu_2O composites prepared at 0.3 M of NaOH(aq) have shown the strongest catalytic performances. Regarding to the highest catalytic activity of the composites with cavities surrounded by CuO flakes, confinement effect is considered to expedite electron transfer from BH_4^- to the dye molecule enormously by reducing the activation energy largely; the energetically favorable formation of the activated complex at the inner walls of a CuO box lowers the energy barrier substantially. In brief, CuO/Cu_2O composites having high catalytic activity have been prepared facilely via a controlled oxidation process of Cu_2O cubes, and they may be applied to treat wastewater in an inexpensive way without employing commonly used noble-metal catalysts.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-15**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photohydroxylation of ZnS nanobelts for enhanced photocatalytic performances

함수호 장두전*

서울대학교 화학부

1D nano-materials like nanorods, nanowires, and nanobelts have been received extensive attention because of their unique properties such as large surface area and high electron transfer efficiency. We have synthesized ZnS nanobelts via a one-pot hydrothermal method. Because ZnS is direct band-gap semiconductor material, the recombination of excited electrons and holes is very fast. To hinder the recombination of charge carriers and to increase the charge-carrier lifetime, we have formed $Zn(OH)_2$ on the surface of the ZnS nanobelts via addition of hydrogen peroxide and Xenon lamp irradiation. By forming the $Zn(OH)_2$ on the surface of ZnS nanobelts, heterojunction between ZnS and $Zn(OH)_2$ have been formed, thus the excited charge carriers have been separated effectively and the lifetime of the excited charges have been increased. We have tested the photocatalytic efficiency of each sample via degradation test of 4-nitrophenol under Xenon lamp irradiation. The optimized sample showed 2.5 times higher photocatalytic activity compared to pristine ZnS nanobelts. Also, we have revealed the photocatalytic mechanism via PL analysis and reactive species tests by using radical scavengers such as p-benzoquinone ($\cdot O_2^-$), EDTA (h^+), and isopropyl alcohol ($\cdot OH$).

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장소: 일산 KINTEX
발표코드: **PHYS.P-16**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

High photocatalytic activity of SnO_2/ZnS nanocomposites

이재원 장두전*

서울대학교 화학부

SnO_2/ZnS nanocomposites of SnO_2 quantum dots (QDs)-deposited ZnS nanorods having highly enhanced photocatalytic activity and photostability have been fabricated via a facile two-step hydrazine-assisted hydrothermal process without involving any surface treatments. The photocatalytic activity of SnO_2/ZnS nanocomposites with a Sn-to-Zn molar ratio ($R_{Sn/Zn}$) of 0.1 is 3 times higher than that of pristine ZnS nanorods and 17 times higher than that of commercial ZnS. The incorporation of SnO_2 QDs increases the photocatalytic efficiency of ZnS nanorods due to the following reasons: photogenerated charge carriers are readily separated owing to type II band configuration and direct contact at interfaces without having any linker molecules; active surface sites are increased to adsorb more dye molecules; the light absorption range is extended to the visible region, generating more charge carriers on the surfaces of heterojunction structures. The decay time, as well as the intensity, of the band-edge emission of SnO_2/ZnS nanocomposites at 325 nm decreases progressively and rapidly with the increase of $R_{Sn/Zn}$, indicating that fast electron transfer takes place from photoexcited ZnS nanorods to SnO_2 QDs. Thus, the higher photocatalytic degradation efficiencies of SnO_2/ZnS nanocomposites are considered to result mainly from the increased separation rates of photogenerated charges. The photostability of SnO_2/ZnS nanocomposites is also improved due to the protection and charge-separation effects of decorating SnO_2 QDs. Our prepared SnO_2/ZnS nanocomposites are suggested to have great potential for photodegradation nanocatalysts in the field of waste-water treatment.

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장소: 일산 KINTEX
발표코드: **PHYS.P-17**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Metal-enhanced photoluminescence of Au_{25} on $Ag@SiO_2$ nanoparticles

김준기 장두전*

서울대학교 화학부

Plasmonic noble metal nanoparticles can significantly interact with closed fluorophores, resulting in fluorescence enhancement. The enhancement relies on near-field enhancement due to SPR induced by metal nanoparticles and is dependent upon the distance between the fluorophore and the plasmonic surface. We report on the metal-enhanced fluorescence of hybrid nanoparticles composed of silver nanoparticles and a promising fluorophore, gold nanoclusters. The photoluminescence spectra of gold nanoclusters-adsorbed to Ag@SiO2 nanoparticles have been investigated systematically with a variation of spatial distances, metal sizes, and excitation wavelengths. The strongest enhancement is observed when the silica shell of the Ag@SiO2 nanoparticle is 6 nm, resulting in an approximately 7-fold increase in emission intensity and a 10-fold increase in quantum yield with a 2-fold reduce in decay time compared to free gold nanoclusters. We have tried to correlate the radiative, metal-modified radiative, nonradiative decay rate with distance-dependence metal-enhanced fluorescence effect. We have also investigated that gold nanoclusters-adsorbed Ag@SiO2 nanoparticles are able to detect heavy metal ions with better sensitive more than free gold nanoclusters.

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장소: 일산 KINTEX
발표코드: **PHYS.P-18**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile self-assembly of silver nanoprisms using polypyrrole for enhanced stability and optical properties

정동원 장두전*

서울대학교 화학부

Silver nanoprisms (AgPRs) have been widely investigated for applications such as solar cells, catalysis, and sensing due to massive electromagnetic field enhancement and high sensitivity, which are attributed to the sharp tips of AgPRs. Herein, we are reporting a one-step polypyrrole (PPy) coating process of self-assembled silver nanoprisms (AgPRs) through the direct polymerization of pyrrole (Py) monomers that also act as an assembling agent. The assemblies of AgPRs, whose edge lengths and thicknesses are typically 78 and 6 nm, have been surrounded by PPy coating of 6 nm. AgPRs are assembled in an edge-to-edge orientation, and the degree of assembly has been controlled by varying the concentration of trisodium citrate which attaches selectively to the {111} facets of AgPRs. Furthermore, the increased red shift of surface-plasmon resonances beyond 930 nm upon increase of the TSC concentration has suggested that the assembly degree of AgPRs can be controlled by varying the concentration of TSC. The morphology deformation time of PPy-coated AgPRs in 0.6 mM H_2O_2(aq) is 7 times longer than that of PPy-free AgPRs, suggesting that PPy coating prevents the sharp tips of AgPRs from being truncated by oxidizing agents. The SERS effect of highly self-assembled and PPy-coated AgPRs becomes as high as 6.3 due to numerous hot spots generated between nanoprisms. Overall, we fabricated AgPRs assemblies with PPy coating which have not only improved structural stability but also enhanced optical properties.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-19**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of morphology-controlled Ag/Au nanocomposites via modified galvanic replacement for enhanced catalytic performances

박태현 이재원 장두전*

서울대학교 화학부

Metallic nanostructures composed of noble metals have received a great deal of research effort due to their potential applicability in variety of fields such as optoelectronics, sensing, bio-labelling, and catalysis which comes from the remarkable structure-dependent properties that are considerably distinct from the bulk-sized ones. Among them, hollow architectures are a particularly interesting class of materials that have unusual chemical and physical properties compared to the respective ones of solid counterparts. Herein, morphology-controlled Ag/Au nanocomposites have been fabricated facilely via a modified galvanic replacement reaction using Ag nanocubes as sacrificial templates. The structures of the Ag/Au nanocomposites produced at galvanic reaction temperatures of 0, 25, 55, 85, and 105 ^{o}C have been found as Au-decorated Ag nanocubes, well-defined nanoboxes, truncated nanoboxes, and porous nanoboxes, and broken nanoboxes, respectively. Compared to pristine Ag nanocubes or Ag/Au nanocomposites without cavities, Ag/Au nanocatalysts with hollow interiors have been found to catalyze the reduction of rhodamine B much more rapidly in the presence of KBH_4. In particular, Ag/Au nanocomposites fabricated at 85 ^{o}C show the most efficient catalytic performances as their largest nanocavities are surrounded by the most porous walls. The high enhancement of catalytic performances is attributed to the facilitation of rapid electron relays from BH_4^- to rhodamine B through the catalytic surface, lowering the kinetic barrier of the catalytic reaction consequently.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-20**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical Evaluation of the Relationships between Structure and Charge Transport Properties in Organic Devices

전병선 이상욱*

한양대학교 바이오나노공학과

Electronic devices based on organic semiconductors have been actively explored for flexible, transparent and low-cost electronic applications. However to realize such applications, the charge transport properties of organic semiconductors must be improved. At the microscopic level, one of the major factors governing the charge transport properties is the amplitude of the electronic transfer integral t, which expresses the ease of transfer of a charge between two interacting molecules. Consequently, the charge transport properties of organic semiconductors critically depend on their molecular packing structures, such as π-π stacking distance and π-π overlap degree. Therefore, tremendous progress toward high-performance organic electronics has been achieved by increasing the charge transport properties through rational design of organic molecules and morphology control of organic crystals. In addition, much attention has been drawn to study charge transport in organic semiconductors in order to find fundamental routes to develop high-performance organic electronics based on an understanding of the intermolecular interactions and the structure-property relationships.Here I demonstrate new approach for controlling organic crystal morphology using eutectic crystallization and provide fundamental understanding of the structure-charge transport property relationships in organic crystals.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-21**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Time-Resolved X-ray Absorption Spectroscopy of Charge Transfer Dynamics of Solvated Ru polypyridyl complex

마로리 김태규*

부산대학교 화학과

Time-Resolved X-ray Absorption Spectroscopy (TR-XAS) is a special tool to investigate molecular dynamics. It also has become possible to observe the transient chemical reactions on fundamental timescale. Ru-based polypyridyl complexes are used in various fields as solar energy conversion, artificial photosynthetic systems and optical sensing. We directly observed the transient ^{3}dd state of ruthenium-based dye molecule, which is $[Ru(m\text{-}bpy)_3]]^{2+}$ (m-bpy = 6-methyl- 2,2′-bipyridine) in liquid phase, by means of ultrafast transient XANES spectroscopy at Ru L3- and K-edge regions at ALS beamline. Besides we performed the time-dependent density functional theory calculations of Ru 2p core-level excitations to visualize the movement of charge density around the Ru atom and the surrounding ligands. To determine the structural parameter changes in Ru-N bond of $[Ru(m\text{-}bpy)_3]^{2+}$ during the ^{3}dd process, we have performed the analysis of transient EXAFS spectra at K-edge region of Ru at KEK beamlime. We find that not only the stabilization of Ru 2p core and 4d valence orbitals, respectively, from L3-edge XANES spectroscopy but also the difference of bond distance of Ru–N and Ru–Nmethyl bonds by 0.01 and 0.03 Å, respectively, from K-edge EXAFS spectroscopy.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-22**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Computational Materials Science for Lithium Ion Battery Materials: Understanding the Degradation Mechanisms of LiNi1/3Co1/3Mn1/3O2

이치호 전병선 이상욱*

한양대학교 바이오나노공학과

Higher energy density combined with longer cycle life is one of the key requirements that need to be addressed in the Li ion batteries applications. Currently, layered Li transition metal oxides were adopted as a power sources for EV and PHEV applications due to their high theoretical capacity and cycling stability. However, accelerated capacity fading still occurs even at the most stable LiNi1/3Co1/3Mn1/3O2 (NCM111). A variety of approaches are being made to find the essential factors affecting the cycling performance. Phase transformation in corporation with a displacement of Li ions from Li layers is known to the crucial features inhibiting the life characteristics of cathode materials, although the mechanisms that drive such evolution at atomic level remain elusive. Here, we present an investigation of chemical and structural evolution induced by Ni migration, and which is the fundamental degradation mechanism of NCM based layered structure cathode materials. This phenomenon was firmly established by combined atom probe tomography (APT) and high-resolution transmission electron microscopy (HR-TEM) analysis. Density functional theory (DFT) calculation was conducted to evaluate the diffusion kinetics of Ni cations within the layered structure and to propose the addition of dopant to suppress the Ni migration.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-23**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Colloidal Quantum Dots with Singly Occupied Higher Quantum State

정주연 윤빛나 정광섭*

고려대학교 화학과

Colloidal quantum dot (CQD) has been rigorously studied for the last three decades due to its tunable optical and electrical properties by varying the nanocrystal size. Since the CQD is semiconducting material, doping density can determine the CQD device performance. Therefore, it is very important to finely control the doping density of the CQD for manipulating the electric, optical and magnetic properties of CQDs. Previous work has shown the tunable intraband transition of mercury chalcogenide CQD by varying the nanocrystal size. Here, we firstly report HgSe CQDs with zero, one (unpaired) or two (paired) electrons occupying the lowest quantum state of the conduction band (1Se), which has been a long-standing challenge in the colloidal nanocrystal research. The number of electrons in the 1Se state is determined by nanocrystal growth time directly involved in the stoichiometry of the metal-chalcogenide CQD. The singly-occupied-quantum-state (SOQS), when an electron fills the 1Se state in stable under ambient conditions, was confirmed by carrying out the electron paramagnetic resonance spectroscopy. Furthermore, the diamagnetism was observed when zero or two electrons are occupied in the 1Se state, corresponding to doubly-occupied-quantum-state (DOQS). Strikingly, superparamagnetism was identified by performing SQUID for the SOQS HgSe CQDs with varying temperature down to 4 K. The number of electrons in the 1Se state, moreover, can be controlled by surface treatment. The SOQS and DOQS of CQD will be a promising magnetic feature for future spin based applications such as nonvolatile memory, infrared optoelectronics, catalysts, optomagneto-imaging and quantum computing.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-24**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Steady-state Mid-Infrared Intraband Transition Occurring in Conduction Band of Heavily Doped Colloidal β-HgS Quantum Dot

윤빛나 정주연 정광섭*

고려대학교 화학과

The mercury chalcogenide colloidal quantum dot (CQD) has been of interest due to the size tunable mid-infrared intraband transition. The first reported absorption spectrum of mercury sulfide CQDs by Jeong et al. in 2014 showed broad size distribution with FWHM over 750 cm^{-1}. The large FWHM apparently mostly results from the non-uniform nanocrystal size. Also, a versatile ligand exchange which is essential for further applications was not achieved from conventional HgS CQD passivated with thiol ligands because of the strong binding strength of the thiol ligands to the nanocrystal surface. Here, we report HgS CQDs passivated with non-thiol ligands offering ligand versatility. In addition, the doping density of CQDs was finely controlled by post surface treatment with ions. The CQD film showing both intraband and bandgap energy depending on the surface treatment, is analogous to the n-p type CQD homojunction. Surprisingly, a novel second intraband transition (1Pe-1De), that had been hidden for the last three decades, was firstly observed from the HgS CQD film by using the FTIR microscope. The combined features of non-thiol passivated HgS CQDs, versatile surface modification, doping control in nanocrystals, and higher quantum state transition hold promise for the use of the heavily doped colloidal quantum dot for a number of applications such as space-communication light source, mid-infrared energy sensitized electrode, infrared detector, and infrared filter.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-25**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Catalytic Reduction of 4-Nitrophenol at Room Temperateres: Boosting Palladium Nanocrystals Efficiency by combining with Copper via Liquid Phaser Plused Laser Ablation

박한빛 **devulapalliamaranathareddy** 마로리 김태규*

부산대학교 화학과

Ultra-dispersed bimetallic nanomaterials have attracted much attention in the hydrogenation of highly toxic aromatic nitro compounds to aromatic amines owing to their high stability, superior activity, reusability, and unique optical and electronic properties, as compared to monometalic nanocrystals. However, the lack of facile and economically controllable strategies of producing highly pure ultra-dispersed bimetallic nanocatalysts limits their practical industrial applications. Considering the above obstacles, we present a simple and effective strategy for the formation of bimetallic (PdCu) nanocrystals by liquid phase pulsed laser ablation using a bulk Pd metal plate submerged in $CuCl_2$ solutions with different concentrations, in contrast to the complex and costly experimental methods used previously. The microstructural and optical properties of the synthesized nanocrystals indicate that the obtained bimetallic nanostructures are highly pure and monodispersed. Moreover, bimetallic PdCu nanostructures show a higher catalytic activity than monometallic Pd and Cu nanocrystals for the hydrogenation of 4-nitrophenol to 4-aminophenol at room temperature, also exhibiting high stability for up to four recycles. The mechanism of the enhanced catalytic activity and stability of bimetallic nanocrystals is discussed in detail. Finally, we believe that the presented design strategy and utilization of bimetallic nanocrystals for catalytic applications enables the development of novel bimetallic nanostructures by liquid phase pulsed laser ablation and their catalytic application for environmental remediation.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-26**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Symmetry-Breaking Charge Transfer in Directly Linked Push-Pull Porphyrin Arrays

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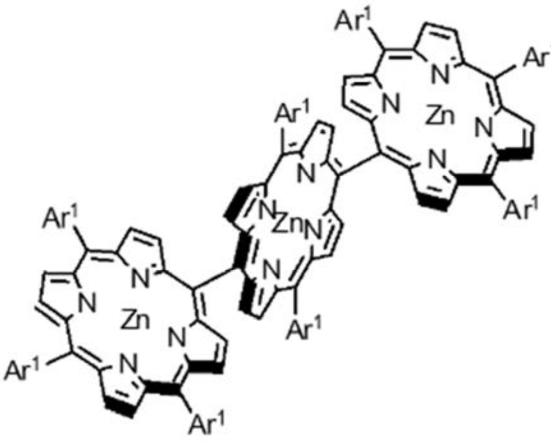
연세대학교 화학과 대학원 [1]연세대학교 화학과

We present symmetry-breaking charge transfer (SBCT) in the excited state with directly linked porphyrin triad (ADA) by spectroscopic results which are of steady-state absorption and fluorescence, time-resolved fluorescence (TRF), femtosecond transient absorption (fs-TA) and time-resolved infrared (TRIR) measurements. Unprecedented broad fluorescence spectra in porphyrin arrays were observed in polar solvents which were attributed to existence of a strong charge transfer state shown via TRF measurement. TA results of triad (ADA) and dyad (AD) showed rising features in excited state absorption (ESA) in polar solvents indicating the formation of a strong CT state which has dipolar sym-metry. This dynamics was also confirmed by TRIR measurement as kinetics was in line with above results providing further information such as solvation and structural relaxation hence those together finally contribute to a relaxed SBCT state. Since this is the first observation of SBCT process among porphyrin arrays, it will provide a fundamental understanding in systems composed of porphyrins, especially for systems composed of strongly coupled moieties. New opportunities for porphyrin arrays will come forward to be used in relevant applications where SBCT is needed.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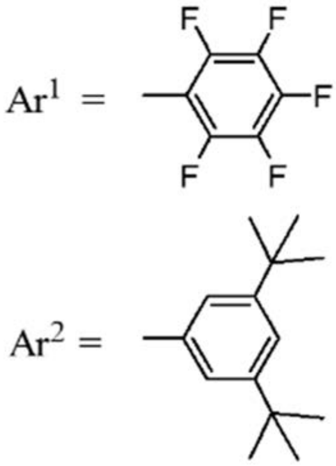
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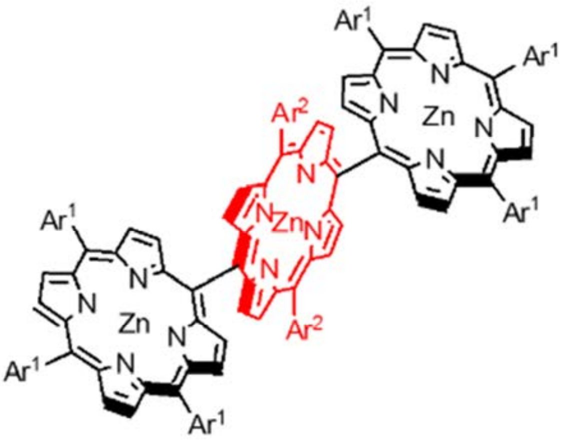
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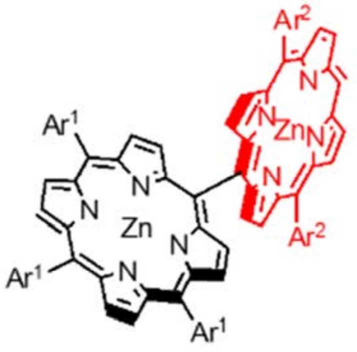
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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-27**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fluorescence studies of the excited-state proton transfer of pyranine in the aqueous sugar and alcohol solutions

홍영호 조한국* 정병서*

인천대학교 화학과

The excited-state proton transfer(ESPT) of a photoacid, pyranine has been studied in the several aqueous sugar solutions. Fluorescence emission from the normal and tautomer forms of the molecule was observed, and the ratios of fluorescence emission intensities of the two forms were measured as a function of sugar concentrations to determine the degree of the ESPT reaction. Comparisons were made with the results in the aqueous solutions of alcohols. Temperature-dependence of the ratio of fluorescence intensities of the normal and tautomer forms was interpreted on the basis of the van't Hoff equation, and the ratio was also correlated with the conductivity of the solution. The dynamic processes of the excited-state proton transfer of pyranine in the sugar and alcohol solutions were discussed.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-28**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Suface-enhanced Raman spectroscopy and density functional theory studies of several phenothiazine dyes adsorbed on silver colloids

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인천대학교 화학과

Surface-enhanced Raman scattering (SERS) spectroscopy was applied to vibrational characterization of thionine and several other phenothiazine dyes adsorbed on silver colloids in order to discern the spectral vibrations among phenothiazine dyes with different methyl substitutions. FT-Raman spectra of powder form of the dyes were also obtained for comparison with the SERS spectra. Density functional theory calculations were performed to aid vibrational assignments of the observed bands and to determine the adsorption structure of dyes on the silver surface. The interaction of dye adsorbates with different methyl substitutions with the metal surface leading to different adsorbate conformations and molecular structures were discussed based on the changes in the observed SERS spectra.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-29**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Autoparameterization of Born-Mayer-Huggins-Tosi-Fumi Interionic Potential for Molten LiCl by Simplified Evolution Strategy

CEDENO RUSHIE MAE 김종윤[1] 이경구[*]

군산대학교 화학과 [1]한국원자력연구원 원자력화학연구부

Improvement of Born-Mayer-Huggins-Tosi-Fumi (BMHTF) interionic potential through autoparameterization using simplified evolution strategy is reported in conjunction with molecular dynamics simulations of molten lithium chloride. The parameters are automatically optimized against the experimental data such as density and ion conductivity at different temperatures. The results show that compared to the old parameters, the obtained new parameters are able to reduce the positive and negative 10-20% errors in predicting the melting point, shear viscosity and ion conductivity of molten LiCl. Thus, the simplified evolution strategy can be a robust algorithmic solution in tuning the potential for obtaining more accurate parameters. This can offer a systematic method significant in computing the experimentally difficult transport properties of molten salts.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-30**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Kinetic Studies of 4-Phenylbenzenesulfonyl Chloride

고한중

전주교육대학교 과학교육과

Solvolyses with the reaction center being the sulfur of 4-phenylbenzenesulfonyl chloride was studied under solvolytic conditions and the extended Grunwald-Winstein equation was applied. The thirty five kinds of solvents gave a reasonable extended Grunwald-Winstein plot with a correlation coefficient of 0.940. The sensitivity values (l = 0.60 and m = 0.47) of 1 were smaller than those obtained for benzenesulfonyl chloride (l = 1.10 and m = 0.61) proposed to undergo dissociative SN2 mechanism. These l and m values for the solvolyses of 4-phenylbenzenesulfonyl chloride can be considered to support a SN2 pathway with some ionization reaction. The activation parameters were determined and they are also in line with values expected for a bimolecular reaction.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-31**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dark Matter miRNA detection using surface-enhanced Raman scattering based on well-designed nanostructure

권혁상

한국표준과학연구원(KRISS) 미래융합기술본부/나노바이오측정센터

MicroRNAs (miRNAs) are small non-coding RNA molecules that have functions in silencing. Recently, the unraveled expression of miRNAs is recognizing as disease states relating with cancer, kidney disease, obesity and nervous system. Herein, we aim to develop ultrasensitive and multiplexed detection platform of miRNAs existing in dark matter of cancer patient no showing therapeutic efficacy for anticancer drug based on surface-enhanced Raman scattering or spectroscopy (SERS). First, we synthesized complementary DNAs with one-end Raman marker and the other-end thiol group, which were self-assembled for the formation of self-assembled monolayer on the SERS substrate with a well-designed nanostructure. Then, we flowed target miRNAs to make DNA:RNA double strands. In this time, Raman signal is “ON” state. To confirm the formation of DNA:RNA duplex through sequence specific hybridization, we finally treated duplex-specific nuclease (DSN) because it has a strong preference for cleaving double stranded oligonucleotides. Once sequence specific hybridization occurs on the SERS substrate, DSN would recognize duplex efficiently followed by degradation of probe DNA, which causes releasing SERS signaling molecule from the surface (“OFF” state). By changing target miRNA with different Raman probes, it will be applicable to the diagnosis of cancer patient based on the dark matter detection under the multiplexed SERS detection.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-32**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoinduced Symmetry Breaking Charge Transfer Dynamics of 9,9'-Bianthracene: Solvent Effects

이창민 주태하*

POSTECH 화학과

Photoinduced symmetry breaking charge transfer (SBCT) is fascinating phenomenon that can be found in biological systems like reaction center of photosynthetic bacteria. Because of its biological importance and applicability, much research about SBCT has been done. 9, 9’-Bianthracene (BA) is a representative model system which undergo SBCT. It has orthogonal torsional angle between two anthracene rings. After photoexcitation, only one anthracene ring is excited and it is called as locally excited state. In polar solvents, charge transfer from one anthracene ring to another ring occurs, making charge transfer state. There is, however, still a lack of understanding about how this reaction is possible and which factors influence it. By obtaining time-resolved fluorescence spectrum of BA in several solvents, it was found that rotational solvation is the most influential factor for the reaction. From the results of the quantum chemical calculation, it is found that the role of the static electric field of solvents is also important in this process.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-33**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dynamics of Hydration Water Plays a Key Role in Determining the Binding Thermodynamics of Protein Complex

정성호 함시현*

숙명여자대학교 화학과

Interfacial waters are considered to play a crucial role in protein-protein interactions, but in what sense and why are they important? Here, using molecular dynamics simulations and statistical thermodynamic analyses, we demonstrate distinctive dynamic characteristics of the interfacial water and investigate their implications for the binding thermodynamics. Molecular dynamics simulations identify the presence of extraordinarily slow (>1,000 slower than in bulk water) hydrogen-bond rearrangements in interfacial water. To elucidate their molecular origin, we introduce the “trapping” free energies of individual hydration water molecules, which characterize how strongly each water molecule is captured by the biomolecular surface. The thermodynamic-dynamic relationship diagram constructed with the hydrogen-bond relaxation times and trapping free energies clearly accounts, in molecular terms, for the emergence of the slow relaxation in the interfacial region upon protein-protein complex formation. We also discuss the impact of the slow interfacial waters on protein-protein interactions by quantifying their contribution to the standard binding free energy. We find that, as expected from their slow dynamics, the conventional approach to the water-mediated interaction, which assumes rapid equilibration of the waters' degrees of freedom, is inadequate. We show instead that an explicit treatment of the extremely slow interfacial water molecules is critical. Our results shed new light on the role of water in protein-protein interactions, highlighting the need to consider its dynamics to improve our understanding of biomolecular bindings.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-34**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dynamics of Counter Ions Surrounding Double-Strand DNA

정성호 함시현*

숙명여자대학교 화학과

Anomalous behavior of counter ions surrounding DNA is a long-standing issue. Recent advances in computer hardware, software, and molecular mechanics force fields have now made it possible to perform atomistically detailed molecular dynamics simulations of sufficient length to obtain reliable description of ion distributions around DNA. However, relatively less attention has been paid to the dynamical aspects of counter ions. In the present work, we investigate the dynamics of counter ions surrounding a double-strand DNA using molecular dynamics simulations. We find that the counter ions in the first shell exhibit extremely slow relaxations occurring on nanosecond timescales, which are comparable to those of the DNA conformational dynamics. Our results indicate the necessity of explicit handling of the first-shell counter ions in the study of DNA, i.e., the counter ions constitute an integral part of DNA.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-35**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Observation of Bond Formation Process via Wave Packet Motion

손소형 주태하*

POSTECH 화학과

Changing chemical bond is the most important process in terms of understanding various phenomena for synthesis and microscopic point of view. Gold is one of the most popular candidate for studying bond formation due to its self-assembly character called aurophilicity. The simplest system of gold, $Au(CN)_2^-$, is used for studying bond formation. There is a controversy about excited state dynamics. Iwamura and his coworker claims that bonds are tightened in excited singlet state and conformational change will occur within ~2 ps using femtosecond pump-probe transient absorption (TA) with ~200 fs time resolution. On the other hand, Ihee group demonstrated intrinsic results about structural point of view using time-resolved X-ray solution scattering (TRXSS). They argue that the bent-to-linear structural change will occur within $_2$ or higher states and triplet states as well as the first excited state. In this regards, time-resolved fluorescence is powerful method which provides information of pure first excited state. Detailed experimental results will be presented in the poster.

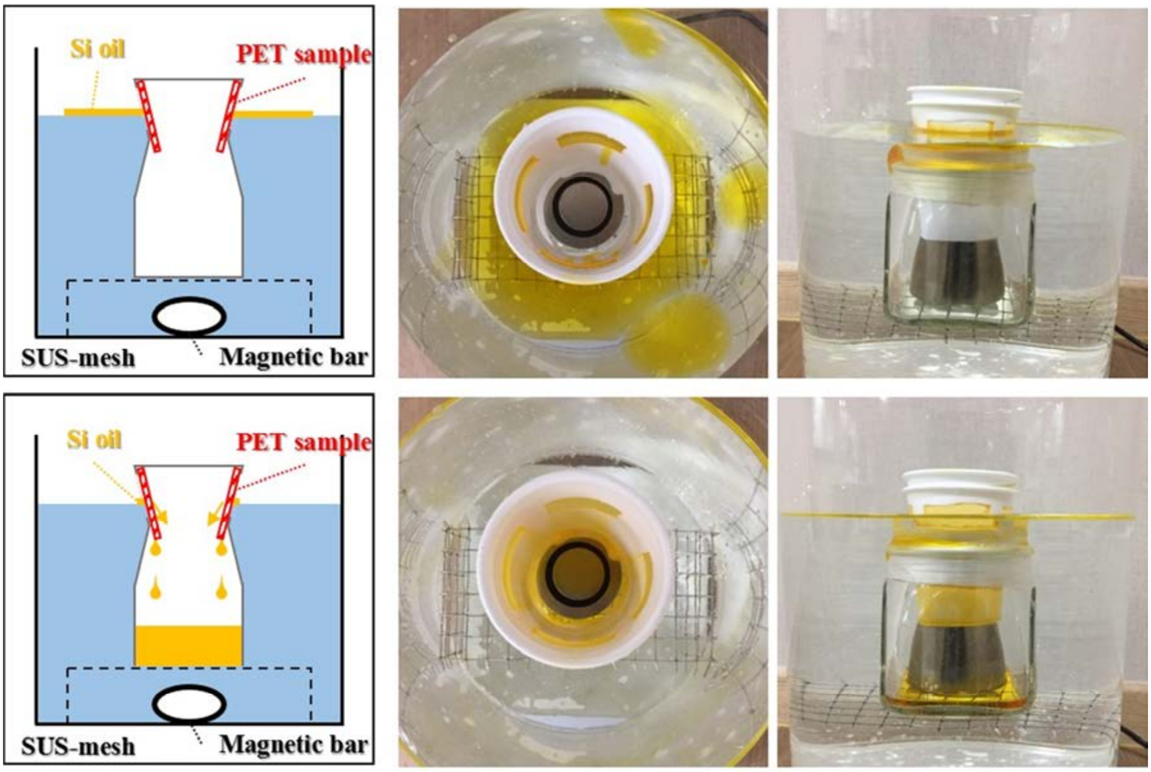
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-36**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fabrication of a Superhydrophobic PET Membrane using PDMS-SiO_2 Nanoparticles: Application in Oil-Water Separation

한상욱 서현욱[1] 김일희 김호종 차병준 박찬흠 정재환 우태균 김영독[*]

성균관대학교 화학과 [1]상명대학교 화학에너지공학과

The commercial polyester (PET) and polypropylene (PP) membrane were coated with polydimethylsiloxane (PDMS)-deposited SiO_2 nanoparticles and they showed a water contact angle greater than 150^o. The adhesion of PDMS-SiO_2 was stronger on PET than PP and it was confirmed with scanning electron microscopy (SEM), Fourier transform-infrared (FT-IR) spectroscopy, water contact angle and water weight gain measurements. The PDMS-SiO_2 coated PET (dip-PET) showed high selectivity towards oil separation from the oil-water mixture, durable hydrophobicity after exposure to strong acidic/basic solutions. It was also demonstrated that the repetitive use of dip-PET for oil-water separation and small scale of oil collecting device using dip-PET as the filter. We suggest that our dip-PET membrane could be used as the cover of oil absorbent pads and oil-water separation filter.


Si oil
PET sample
SUS-mesh
Magnetic bar
Si oil
PET sample
SUS-mesh
Magnetic bar

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-37**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Composition-dependent quantum-confined Stark effect in lead bromide perovskite nanocrystals

함수진 정희재 김동호*

연세대학교 화학과

We present a study the origin of the emission linewidths broadening observed for lead bromide ($APbBr_3$, A = CH_3NH_3 and Cs) perovskite nanocrystals (NCs). Our analysis is based on a statistically significant number of nanocrystal spectra and defocused images measured by confocal and wide-field microscopy, respectively. Based on this observation, we explain the particular susceptibility of $CH_3NH_3PbBr_3$ NCs to spectral diffusion causing the linewidth broadening via the linear quantum-confined Stark effect. After laser excitation and exciton formation, an electron or hole from the exciton localizes near the surface of the NC leaving a delocalized charge carrier inside the NC core. Following this initial charge localization or ionization, the delocalized charge carrier can also be localized leading to a net neutral NC core. If the NC environment is decorated by charges following previous process, then after subsequent ionization, a charge localized in the NC's environment can relax back into the NC core recombining with the delocalized charge carrier. These mechanisms would create, if not alter, a surface dipole and lead to a net change in the local electric field. The single NC spectra express this change as a large Stark shift in the emission frequency. This comparative investigation of $CH_3NH_3PbBr_3$ and $CsPbBr_3$ NCs enable us to understanding the relationship between polarity of NC and emission linewidths broadening of lead bromide perovskite nanocrystals.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-38**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Binding interaction of propyl gallate with bovine and human serum albumins by fluorescence spectroscopy

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인천대학교 화학과

The interaction of the antioxidant, propyl gallate (PG) with bovine and human serum albumins in phosphate buffer has been studied by fluorescence spectroscopy. The intrinsic fluorescence of serum albumins was monitored as a function of PG concentrations. Fluorescence quenching assays were used to characterize the binding affinity of PG. The fluorescence quenching constants were determined based on the Stern—Volmer and modified Stern—Volmer equations. In addition, the binding constant and the number of binding sites between serum albumins and PG were determined by the Scatchard-type analysis. The site marker displacement experiments were performed to identify the binding site of serum albumins using warfarin and ibuprofen as site markers.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-39**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Induced Circular Dichroism of Jet-cooled Phenol Complexes with Chiral Solvents

홍아람 민아름[1] 문철주[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 various chiral solvents using resonant two-photon ionization spectroscopy (R2PI). The R2PI spectra of phenol complexes exhibit well-resolved vibronic bands of the 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 correlation between the structures of the complexes and ICD effect will be discussed.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-40**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Conformation-dependent Rebinding Dynamics of CO with Myoglobin Investigated by Time-resolved Infrared Spectroscopy

신주향 임만호* 박성철

부산대학교 화학과

Myoglobin is one of the simplest heme proteins and has been studied extensively using a variety of physical techniques. In this study, we have measured the ground state bleaching of MbCO at low pH using time-resolved vibrational spectroscopy. When excited with a 532-nm photon, carbon monoxide dissociated immediately from myoglobin (< 0.2 ps), ground state bleaching of CO bound to the myoglobin has three conformations (A0, A1 and A3). Each conformation shows characteristic ^{13}C−O stretching frequencies : 1920 cm^{-1} for A0, 1990 cm^{-1} for A1 and 1896 cm^{-1} for A3. Ligand binding to myoglobin is a multiphasic process with fast geminate rebinding arising on the nanosecond timescales and slower bimolecular rebinding occurring on microsecond timescales.We have observed faster geminate rebinding time and bimolecular rebinding time for A0 than the others.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-41**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Simulation Study on the Structural Motif and the Translation-Rotation Decoupling in Glass-Forming Liquids

박윤재 성봉준*

서강대학교 화학과

Glass transition, which is a transition from liquid to amorphous solid, has been investigated for ages. There is, however, no consensus on the origin and the nature of the glass transition. Some suggest that the glass transition should result from a kinetic trap while others argue that a structural motif exists and plays an important role according to a thermodynamic viewpoint. In this work, we investigate the presence and the effect of the structural motif upon the glass transition by employing tracers, especially their translation-rotation decoupling behaviors. Because of the lack of structural information in 3D glass formers, it is hard to identify the local structural motif. Here, we use the topological cluster classification to identify the energy minimum clusters and perform molecular dynamics simulations of Wahnström binary Lennard-Jones colloids with tracers of three different shapes, i.e., icosahedron, FCC, and HCP. For icosahedron tracers, a long-lived locally favorable structure, the translation-rotation decoupling occurs and the high fraction of neighboring particles of the same structure suppresses the rotation more compared to the translation. For other types of tracers, the decoupling is not significant compared to the icosahedron tracer. The difference in the decoupling behavior between different types of tracers indicates that there should be the structural motif during the glass transition.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-42**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular Self-Assembly and Phase Transition of 2,4-Dichlorobenzenethiol on Au(111) Surface

성시천 노재근*

한양대학교 화학과

Self-assembled monolayers (SAMs) are ultrathin film of organic molecules which are usually consist of head group, backbone spacer and terminal group. They are useful tools for tuning surface properties. Especially, SAMs having aromatic backbone structure with electronegative halogen atoms are useful in electrical applications because of their ability to modify energy barrier of metal surface. Since this energy barrier of surface is significantly affected by density and orientation of the molecular monolayer, it is important to illuminate the packing structure of SAMs. In our previous studies, fluorinated aromatic thiol SAMs showed closely packed domains with intrinsic and specific structures, and its orientation was strongly affected by dipole-dipole intermolecular interactions which are oriented from location of electronegative halogen moieties. Among them, size of ordered domains of 2,4-difluorobenzenethiol (2,4-DFBT) SAMs was overwhelming. In this study, 2,4-dichlorobenzenethiol (2,4-DCBT) was used to confirm dipole-induced organization of halogenated aromatic molecules, which are readily shown in the fluorinated adsorbates. The 2,4-DCBT SAMs was deposited at high temperature (~ 363 K) under atmospheric condition, and characterized by scanning tunneling microscopy (STM) and cyclic voltammetry (CV) to investigate structure and electrochemical behavior of the SAMs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-43**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Formation and Structure of Benzeneselenolate Self-Assembled Monolayers on Au(111) Derived from Benzeneselenocyanate and Diphenyl Diselenide

한슬기 이남경 노재근*

한양대학교 화학과

Self-assembled monolayers (SAMs) of organic thiol on gold substrate have been extensively studied due to their various potential applications such as nanolithography, nanoscience, molecular recognition, bioscience, and electronics. Nowadays, thiosulfates, thiochlorides, thiocyanates, and selenium group are regarded as a promising material in the preparation of SAMs due to their higher oxidation stability than organic thiols. Molecules containing a pi-conjugated system have been much researched due to their useful as a molecular junction. In this work, we compared the formation and structure of SAMs on Au(111) from benzeneselenocyanate (BeSeCN) and diphenyl diselenide (DPDSe) by ambient-pressure deposition. The adsorption of BeSeCN and DPDSe on Au(111) results in the formation of benzeneselenolate SAMs on Au(111) through the cleavage of Se-CN and Se-Se bond, respectively. Both SAMs were composed of many adatom islands, as found in aromatic thiol SAMs. Scanning tunneling microscopy imaging revealed that the ordered domains of DPDSe and BeSeCN SAMs have a $(3\sqrt{2} \times \sqrt{43})$ and $(\sqrt{3} \times \sqrt{5})$ packing structure, respectively.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-44**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Nanoscopic Investigation on Formation of Unsymmetric Adamantyl Alkyl Disulfide Self-Assembled Monolayers on Au(111)

손영지 한슬기 노재근*

한양대학교 화학과

Self-assembled monolayers (SAMs) formed by organic molecules containing sulfur headgroup on metal surfaces have drawn much attention because of its ability to control the physical and chemical properties of solid surface. In nano and biotechnology, symmetric or unsymmetric dialkyl disulfides have been often used for the fabrication of molecular thin fillmes to adjusting the degree of phase segregation and preferential adsorption. However, there have been no reports on the domain formation and strcuture of unsymmetric adamantyl hexyl disulfide (AHDS) and adamantyl decyl disulfide (ADDS) containing adamantyl group with aliphatic 3D carbon cage structure and normal alkyl chains on Au(111) from the molecular-scale viewpoint to date. In this study, we have monitored the formation and domain strcuture of AHDS and ADDS SAMs on Au(111) using scanning tunneling microscopy. We revealed the unique ordered domains of these SAMs on Au(111), which have never been observed from each single component SAMs from 1-adamantanethiol, 1-hexanethiol and 1-decanethiol using molecular-scale scanning tunneling microscopy.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-45**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Hofmeister anion effect for water network near protein surface

이의현 조민행*

고려대학교 화학과

We have focused on the water in protein interface using MD simulation. Go further we investigated the change of water network at interface under the ionic condition to understand the ion effect near protein surface. The H-bond number of water is the criteria which represents water network, already there are many researches about H-bond number along distance from hydrophobic surface such as protein and graphite. The collapse of water network is observed near protein surface from our results through the decrease of H-bond number. Under ionic condition, H-bond decrease patterns are revealed differently along the Hofmeister anion series which is related with solubility of protein near protein surface while there are no specific ion effects over 5 Å region. This result has relation with ion distribution. Chaotropic anions showed higher preference near protein surface than kosmotropic anions. Additionally, we investigated the number distribution and orientation distribution of each configuration of water to confirm preferential orientation at organic phase/water interface. Our results showed that the water has mainly random distribution, but slightly there are preferential configuration for straddle structure at protein/water interface.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-46**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A miniature split/splitless liquid injection system for portable GC

유동욱 정광우* 방주연

원광대학교 화학과

Split and splitless injections are gas chromatographic techniques that introduce the sample into a heated injection port as a liquid, and then rapidly and completely vaporized the sample solvent as well as all of the analytes in the sample. The vaporized sample is transferred to the head of the GC column. This work demonstrates a miniature split/splitless injection system for quantitative determinations of liquid sample mixtures in GC analysis. The injector temperature is adjustable from ambient to 300℃. The split flow is adjustable by means of flow/pressure sensors and a precision proportional valves. System performance will be discussed in terms of the selectivity and sensitivity of GC separation. Split/splitless injector is expected to be used for a portable GC instrumentations.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-47**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A portable GC-PID system for monitoring of air pollution

유동욱 정광우* 방주연

원광대학교 화학과

Current study describes a portable GC (30×20×15 cm3, 5 kg) for real-time and quantitative determinations of gas mixtures in air sample. This system is integrated with a low thermal mass column module, electronic pressure controller, and a miniaure photoionization detector. Ambient air is employed as a carrier gas, and a diaphragm pump is used to provide the pressurized carrier gas. Based on the experimental results, the system can effectively separate and detect the trace amount of air pollutants within 10 min. The results show that this portable GC-PID can be widely applied to the on-site detection, including indoor air quality, industrial emission control, rapid detection of explosives in public place, and breath analysis.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-48**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of carbon nanotube sponges

방주연 정광우* 유동욱

원광대학교 화학과

In this research, we synthesized carbon nanotube (CNT) sponge which has porous, uniform, soft, flexible and freestanding structure. The growth process of CNT sponge is based on liquid-injection chemical vapor deposition (CVD) with a quartz tube as a reactive chamber. Ferrocene and 1,2-dichlorobenzene were used as the catalyst precursor and carbon source, respectively. Also, injection system of carbon sources is operated by using a spray nozzle unlike other experimental methods of previous literatures. Physical characterization of the CNT sponge such as porosity, adsorption property, superhydrophobicity and surface morphology was verified. Synthesized CNT sponge has numerous interesting properties which may make it useful for a variety of applications, including supercapacitors, energy storage, environmental materials and concentrator.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-49**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Investigating emitter orientation in host-guest films with angle-dependent photoluminescence (PL) measurement

이준호 이치호 박성남*

고려대학교 화학과

Small molecule organic light-emitting diodes (SM-OLEDs) have been developed as a distinctive device. So far, a low outcoupling efficiency has still been a challenge to enhance the external quantum efficiency (EQE), even though the intrinsic quantum efficiency reaches almost 100%. One of the suggestion to increase the outcoupling efficiency in amorphous SM-OLEDs is implementing horizontally oriented emitters inside host molecules. In the case of a host-guest system which has been commonly used in thermally activated delayed fluorescence (TADF) OLEDs, and phosphorescence OLEDs (Ph-OLEDs), angle-dependent PL measurements have been used to determine the molecular orientation. Moreover, two anisotropic refractive indices which are obtained by variable angle spectroscopic ellipsometry (VASE) measurements are required for a determination of emitter orientation as fitting parameters. In this work, instead of using uniaxial refractive indices determined from the VASE, we propose an alternative method using an effective refractive index to fit angle-dependent PL data. Employing this method, we have verified that the molecular orientation of dopants is not dependent on the film thickness and the high aspect ratio of dopant molecules is a major factor to give the horizontal orientation of dopants. Overall, our present method is shown to be reliable and thus it is utterly promising to examine the molecular orientation of emitters in various host-guest systems.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-50**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study of non-resonant effects of Stimulated Raman Scattering with intensive Raman pump pulse

임소희 천봉환[1] 이한주[2] 조민행[*]

고려대학교 화학과 [1]IBS CMSD & 고려대학교 화학과 [2]한국기초과학지원연구원 서울센터

Unlike spontaneous Raman effect, stimulated Raman scattering (SRS) generates fields allowing Raman signals from individual scatterers to add up into a highly directional, high-brightness coherent beam. In our experiment, however, at intensive Raman pump energy, the SRS spectra is distorted dramatically. The experimental results are compared with theoretical simulation by numerically solving the third order susceptibility. These results show that nonlinear effects such as XPM, SPM can be included in SRS signals with intense Raman pump pulse. It will be presented to discuss about the characteristic dispersion-shaped SRL signals related to XPM.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-51**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Water and Ion Effects on the Stability of Human Telomeric DNA G-quadruplexes by Molecular Dynamics Simulations and Solvation Thermodynamics Analyses

이진경 함시현*

숙명여자대학교 화학과

Specific 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 propeller, antiparallel basket, mixed-hybrid 1 and mixed-hybrid 2) of Human telomeric G-quadruplexes depend on environmental factors, the relative stability of those structures remains elusive. Here we investigate the molecular origin on the stability of Human telomeric G-quadruplexes to know the conformational preference, with 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 solution upon Human telomeric G-quadruplexes.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-52**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical study about the formation of two-dimensional molecular network on Au(111)

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We investigated self-assembly of (S)-β-benzyl-γ-aminobutyric acid, rationally designed amino acid, on Au(111) using density functional theory calculations. The ring-shaped cluster at low coverage is stabilized by intra- and intermolecular hydrogen bonding between ammonium and carboxylate group. The degree of stabilization depends on the number of self-assembled molecules, and the hexamer is the most favorable among various self-associated molecular clusters. The change of the ring-shaped cluster into two-dimensional molecular domains at monolayer coverage was also investigated. Theoretically simulated STM images from the optimized molecular network are consistent with experimentally observed features.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-53**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Interferometric Scattering Microscopy (iSCAT)

주종현 조민행*

고려대학교 화학과

We can observe microscopic world with optical microscope. As techniques for imaging are developed, we can get images of nano-sized particles and molecules with high spatial resolution. Unfortunately, super-resolution imaging techniques using fluorescent molecules suffer photobleaching or photoblinking because lifetime of fluorophore is limited. However, detecting nanoparticles using interference of scattered light by themselves, we can directly observe dynamics of nano-materials with high time resolution as well as overcome time limit of fluorescence imaging. In this work, we constructed optical system of interferometric scattering microscopy (iSCAT). Using iSCAT, we got images of gold nanoparticles with 40 nm diameter and analyzed time trace of their movement.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-54**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Transition metal doped Molybdenum Sulfide (M-MoS_2) Ultrathin Nanosheets as Co-catalyst for Photocatalytic Hydrogen Production via Water Splitting

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부산대학교 화학과

Transition metal dichalcogenides(TMDs) semiconductors are studied to apply to co-catalyst for photocatalytic hydrogen evolution reaction(HER) via water splitting. Due to its 2D layer structures, it has a structural stability and also can help to separate photo-excited charge carriers. Among these semiconductors, molybdenum sulfide(MoS_2) is one of the most promising candidate, because it can be replaced noble-metal and is earth-abundant. Our previous work, loading liquid exfoliated ultrathin monolayer MoS_2 onto CdS nanorods was confirmed that it has amazingly higher efficiency for photocatalytic HER than bulk MoS_2, because of broadened surface and more exposed active edge site. To enhance photocatalytic effect, we synthesized transition metal(M = Fe, Co, and Cu) doped MoS_2 and confirmed photocatalytic efficiency. Transition metal doping effect is expected that it can control conduction band of MoS_2. As a result, M-MoS_2 is a more effective co-catalyst for HER than MoS_2. Especially Cu doped MoS_2 was demonstrated the highest efficiency among four metals. The optimized Cu-MoS_2/CdS exhibited more higher hydrogen production rate about 194.18 $mmol \cdot h^{-1} \cdot g^{-1}$ than MoS_2/CdS that has production rate of 130.0 $mmol \cdot h^{-1} \cdot g^{-1}$. And we checked its durability and analyzed the its properties with various characterization techniques.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-55**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design of self-transforming nanosheets to helices

윤상희 심은지*

연세대학교 화학과

Soft helical nanostructures based on organic moieties can be obtained by self-assembly. Utilizing dissipative particle dynamics simulations with coarse-grained models, we program two-dimensional layer nanosheets with defects to self-roll into hollow helices or helix-like nanostructures. We show that the helical secondary structure can be controlled by defect patterns and densities. The sheet consists of lyophobic beads and simulation box was filled with theta solvent. Therefore, defected side causes anisotropy to the sheet self-transformation into a helix or a helix-like structure spontaneously. Self-rolled structure’s radius and pitch are controlled by varying the defect width and the defect density.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-56**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Disorderly synthesized nanocrystals with Disordered distribution cause Disorder energy

오태환 심은지*

연세대학교 화학과

We investigated the energy disorder in semiconductor nanocrystal (NC) systems. The energy disorder in nanocrystals is recognized as one of the key issues in controlling the carrier mobility in nanocrystals. For potential applications of granular electronic materials in electronic and optoelectronic devices, understanding the properties of semiconductor NCs has drawn much attention. However, the characteristics of NCs is largely affected by the polydispersity of NCs and, thus, it is important to explore the role of the energy disorder caused by the size disorder. We evaluate the energy disorder by employing the lognormal size distribution model and discuss the influence of the polydispersity on the carrier mobility of NC systems.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-57**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optoelectronic studies of Bare and Ligand capped CdSe

김효진 심은지*

연세대학교 화학과

In this presentation, we focus on the relationship between white light emission of CdSe nanoparticles and composition/coverage of ligands. In experiments, some ligands including trioctylphosphine oxide(TOPO), phosphonic acid, and amine have been reported to quench the broad trap state emission, whereas thiols raise the intensity of the trap state emission. This observation suggests that the regulation of white light emission is possible by means of ligand exchange, which certainly has been realized in experiments. However, fundamental understanding for the relationship between the ligand properties and the quenching/enhancement of the trap state emission has not been clarified yet. We employ density functional theory to investigate the role of ligands on the electronic structures of CdSe nanoparticles in presence or absence of various ligands. We show that the band gap structure, hence, the white light emission can be controlled by manipulating ligands not only by their distinctive chemical properties but also by the composition and the coverage of ligands.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-58**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular structure and dipole moments of 2-fluorophenylacetylene analyzed by microwave spectroscopy

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The rotational spectra of the parent and eight 13C isotopomers of 2-fluorophenylacetylene have been measured by chirped-pulsed Fourier-transform microwave spectroscopy in the frequency range of 6-17 GHz. The rotational constants for the parent isotopomer were determined by AABS package program. The dipole moments has been obtained by the Stark effect measurement in the voltage range of +-5 kV. The bond lengths and angles are obtained from the least-squares fitting method and compared to the structure from Kraitchman substitution equation. These experimental structure and dipole moments were compared to the *ab initio* structure.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-59**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Exploring the Buried Interface: Electronic Sum-frequency Generation (ESFG) Spectroscopy on Polymer/Substrate Boundaries

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서울대학교 생물물리 및 화학생물학과 [1]서울대학교 화학부

One of the most important and interesting photonic technologies emerged recently is a device that utilizes interconversion between an electrical charge and photon, as clearly demonstrated by examples such as light-emitting diodes (LED) and solar cells. Numerous phenomena crucial to the workings of such devices occur at the interface between two layers. However, difficulty in probing the "buried" interface without damaging materials makes it challenging to investigate the interface *in situ*. ESFG spectroscopy is a 2nd-order nonlinear optical spectroscopy that can probe only the interfacial region intrinsically by its symmetry-forbidden nature, thus enabling the selective analysis of the electronic structures of the interface while causing no sample damage. In this study, we investigated various polymer/substrate interfaces as a model of organic semiconductor devices by ESFG spectroscopy, in order to unravel correlations that exist between interfacial electronic structures and other parameters.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-60**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

NaCl and KCl Salt Effect on the Memory Time of Magnetized Water

이성현 전상일*

강릉원주대학교 화학과

많은 기능수(functional water)들의 가장 큰 문제점은 재현성의 부족과 짧은 memory time 이다. 일반적으로 NaCl 과 KCl 은 물분자의 구조에 영향을 미치는 염들이다. Na+ 이온은 물분자의 구조 형성 이온이며, K+이온은 물분자의 구조 파괴 이온으로서 상반되는 효과를 보인다. 자화수(magnetized water)는 원래 물분자가 자화 되어서 자기장의 특성을 갖는다는 의미가 아니라, 자기장에 의하여 물분자 배열이 바뀌어져서 특이한 물의 특성을 보이는 상태를 의미한다. 자화수는 물 분자가 더 조밀하게 구조화되어 작은 cluster 들을 많이 형성함으로써 반응성 및 용해도가 증가됨을 보인다. 본 연구에서는 증류수를 자화처리 한 자화수(MW), 증류수에 1 wt% 이하의 염(NaCl, KCl)을 첨가한 후 자화처리 한 자화수(I-MW), 증류수를 자화처리 한 후에 1 wt% 이하의 염(NaCl, KCl)을 첨가한 자화수(MW-I)를 비교 측정함으로써, 첨가된 염이 자화수의 memory time 에 어떠한 영향이 있는지를 전도도, 표면장력, IR 측정 방법을 이용해 알아보고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-61**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Spin relaxation of various ligand coated ultrasmall Gd_2O_3 nanoparticles: effect of ligand-Size and ligand-chain hydrophilicity

tirusew tegafaw 이강호*

경북대학교 화학과

In this work, we synthesized water soluble and biocompatible ultrasmall Gd_2O_3 nanoparticles coated with various ligands were investigated. These ligands include small diacids with hydrophobic chains, namely, succinic acid, glutaric acid, and terephthalic acid, and large polyethylenimines (PEIs) with hydrophilic chains, namely, PEI-1300 and PEI-10000. Ligand-size and ligand-chain hydrophilicity effects were observed. The r_1 and r_2 values generally decrease with increasing ligand-size.The structural, morphological, surface coating, toxicity and their application are studied.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-62**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Ultra-thin MoS_2 layers anchored exfoliated reduced graphene oxide nanosheet hybrid as a highly efficient cocatalyst for CdS nanorods towards enhanced photocatalytic hydrogen production

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부산대학교 화학과

The development of novel highly efficient noble metal-free co-catalysts for enhanced photocatalytic hydrogen production is of great importance. Herein, we report the synthesis of novel and highly efficient noble metal-free ultra-thin MoS_2 (UM) layers on exfoliated reduced graphene oxide (ERGO) nanosheets as a cocatalyst for CdS nanorods (ERGO/UM/CdS). A simple method different from the usual preparation techniques is used to convert MoS_2 to UM layers, graphene oxide (GO) to ERGO nanosheets, based on ultrasonication in the absence of any external reducing agents. The structure, optical properties, chemical states, and dispersion of MoS_2 and CdS on ERGO are determined using diverse analytical techniques. The photocatalytic activity of as-synthesized ERGO/UM/CdS composites is assessed by the splitting of water to generate H_2 under simulated solar light irradiation in the presence of lactic acid as a hole (h^+) scavenger. The observed extraordinary hydrogen production rate of ~234 $mmol\bullet h^{-1}\bullet g^{-1}$ is due to the synergetic effect of the ultrathin MoS^2 layers and ERGO, which leads to the effective separation of photogenerated charge carriers and improves the surface shuttling properties for efficient H_2 production. Furthermore, the observed H_2 evolution rate is much higher than that for individual noble metal (Pt), ERGO and MoS_2-assisted CdS photocatalysts. Moreover, to the best of our knowledge, this is the highest H_2 production rate achieved by a RGO and MoS_2 based CdS photocatalyst for water splitting under solar light irradiation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-63**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Excitonic structure of the FMO complex from molecular dynamics simulations with realistic atomistic chromophore potentials

김창우 이영민*

POSTECH 화학과

Energy transfer dynamics in Fenna-Matthews-Olson (FMO) complex has been extensively studied as a simple prototype model of photosynthetic light harvesting process. Due to the large burden of quantum chemical calculations, most of the studies have relied on abstract models, and atomistic level of treatments are rare. Recently, we have developed a reliable atomistic potential energy model for the bacteriochlorophyll a units in the FMO complex. Molecular dynamics simulations with our potential energy surface based on interpolated mechanics/molecular mechanics(IM/MM) technique allow us to easily investigate physical aspects over nanosecond-timescales while maintaining nearly quantum chemical accuracy. From these, we extracted time-dependent site energies and electronic couplings and converted them into excitonic energies under the scope of the Frenkel exciton model. In particular, the spectral density of the lowest excitonic level was obtained by mimicking the experimental condition and compared with experimental results. We also calculated the Stokes shift of each site from direct excited state simulations, which revealed that the widely used harmonic bath model is reliable for the FMO complex.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-64**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

The cell penetrating TAT-peptide coated ultrasmall Gadolinium-oxide nanoparticle for Water Proton Relaxivity and In-vitro T_1 MR imaging

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경북대학교 chemistry [1]경북대학교 화학과

Gadolinium (III), with its high electron magnetic moment, is the most common T_1 contrast agent, that provides nonspecific positive T_1 contrast. We hereby propose a synthesis for TAT peptide coated ultrasmall Gd_2O_3 NPs, in a facile one pot synthesis. The large relaxivities of TAT-GNPs were observed in aqueous sample solutions (r_1= 18.2 s^{-1}mM and r_2=30.2 s^{-1}mM), as a viable tool for T_1-MRI. The performance of nanoparticles for biomedical applications is highly dependent on the nature and quality of surface coating materials. In this study, the coating of TAT-peptide on the surface of Gd_2O_3nanoparticles were confirmed by FT-IR.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-65**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Reaction between molybdenum and hydrogen sulfide in gas phase

남승수 심은지*

연세대학교 화학과

Transition metal dichalcogenides, especially MoS2, is now attracting attention as a two-dimensional material with considerable band gap and reasonably high carrier mobility. The most widely used method for synthesizing MoS2 is chemical vapor deposition. Although numerous techniques for the chemical vapor deposition of MoS2 have been reported, there has been no report on the molecular-level reaction mechanism present in the chemical vapor deposition method. Here, using density functional theory, we have studied the early stages of MoS2 formation. By calculating the stability and energy for various intermediates in the form of MoSxHy formed by the reaction of Mo and H2S, we found a plausible gas phase reaction pathway that leads to solid MoS2 formation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-66**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effective Reduction Potential Tuning by Functionalization on Ligand Sites Determined via Molecular Orbital DFT Calculations

FRANCIS KIRBY BURNEA 임종현 남연식 이진용*

성균관대학교 화학과

We systematically investigated the tuning of the reduction potentials (E0) for the first row transition metal (M = Cr, Mn, Fe, Co, Ni) complexes with the functionalized 1,4,7-Triazacyclononane-N,N',N"-triacetate (TCTA) ligands by means of DFT calculations. To predict reliable E0, the modified UB3LYP functional and equilibrium concept between high and low spin states were utilized. The functional groups –NH2, –CN, –F, and –NO2 were attached to the carbon atoms carefully selected by considering the LUMO and steric hindrance. Based on firmed accuracy of DFT calculations, finally we obtained the calculated E0 for a series of complexes. It was found that electron donating group such as –NH2 will cause a negative shift of E0 while electron withdrawing groups have the opposite effect. The overall trend of the calculated E0s according to ligand modifications were predicted to have the order as -NH2 < Pristine < -F ≈ -CN < -NO2. In addition, optimized geometries, LUMO, vertical electron attachment and energy components constituting E0 were discussed in detail to assist the further understanding for E0s. Consequently, we suggested that 16 complexes can play a role as a catholyte in aqueous redox flow battery. They can be classified into 5 groups having similar E0 ranges: Group I (- 0.6 V ~ - 0.7 V), Group II (around 0.0 V), Group III (around 0.3 V), Group IV (0.6 ~ 0.8 V) and Group V (1.1 ~ 1.2 V). Especially, it is expected that [MnLF], [MnLCN] and [NiLNH2] can be used as promising catholyte candidates possibly possessing high E0s which almost reach to the reduction potential limitation 1.25 V in aqueous redox flow battery. Our systematic approach to tune E0 can be applied to the design other complexes via rational ligand modification.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-67**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

3D Chemical Database as Workbench with Spark and Django

정다운 조광휘*

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The 3D chemical database is important in the field of drug development or engineering new materials. Essential conditions of the good molecule database are having many entries with correct structures without duplications and including the fast and convenient retrieval system. Pubchem is the big and excellent database we usually use. There are not only a number of 3D molecule data but also a number of 2D molecules without 3D information. We made the 3D database which has 3D coordinates data completely and essential conditions for the good molecule database. We gathered all 2D & 3D molecule data from pubchem database and converted to 3D molecules. YaChI which is the most precise discrimination format was used to remove the duplicated molecules. We used the django as basic web framework and improved the searching speed with the spark distributed system. We constructed the searching & storage system and combined the workbench which enable that people can use the results of searching on the web environment. Plus, database UI can be changed according to the display of instruments user uses. We believe that our 3D chemical database will be a more help to scientists who are researching QSAR or QSPR than other databases.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-68**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Spatial Control over the Formation of Gold Nanoparticle Assemblies

이성운 윤상운*

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Plasmonic nanoparticles represented by gold nanoparticles (AuNPs) exhibit unique optical properties. Surface plasmon resonance (SPR) leads to enormously large absorption or scattering of visible light, localized electric fields around the nanoparticles, and local heating of the medium surrounding of the nanoparticles, permitting a wide variety of applications of AuNPs. Nanoassembly systems consisting of these AuNPs offer many more advantages over the individual nanoparticles. Plasmonic resonances are easily tunable using the nanoassemblies simply by changing the interparticle distances, relative orientations, and the shape, size, and composition of their constituent nanoparticles. Interstitial gaps, naturally formed in the nanoassemblies, provide hot spots where electric fields are greatly intensified. For many applications, it is often required to address the nanoassembly systems in a location specifically needed. However, spatially controlled assembly of nanoparticles is challenging. Electron beam lithography or scanning probe micriscopy is unsuited to fabrication of assemblies in a large scale. Deposition of colloidal dispersion of nanoparticle assemblies onto a micrometer-scale pattern is highly unlikely. In this presentation, we demonstrate that we can form AuNP assemblies on a glass or gold substrate at any desired spots in a micrometer-scale spatial resolution. For this, we exploit the photooxidative desorption of thiol linkers by UV irradiation. The results are applied to color patterning and a design of SERS-probing microchannels.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-69**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Aromaticity Reversal in the Excited Triplet State of Archetypical Möbius Heteroannulenic Systems

오주원 김동호*

연세대학교 화학과

Aromaticity plays a key role to explain various molecular properties. Now, much attention on the aromaticity has been moved from the ground to excited state and its application because the verification of excited state aromaticity not only rationalizes the photostability and photoreactivity but also facilitates designing photoactive materials such as saturable absorbers. Particularly, in light of the excited state aromaticity, the comprehension of molecular structural change and (de)stabilization upon irradiation enables us to reveal photosynthetic mechanisms and expand their synthetic applications. The excited state aromaticity, for the lowest triplet (T1) state, was first described by Baird. He proposed that Hückel aromatic and antiaromatic characters are reversed in the T1 state into antiaromatic and aromatic ones, respectively (known as Baird’s rule). In line with this pioneer work, numerous efforts have been devoted with high-level quantum calculations and experimental observations to describe aromaticity in the T1 state. In this respect, we explored aromaticity reversal in the T1 state of a comparable set of Hückel/Möbius aromatic expanded porphyrin congeners by optical spectroscopy. In the T1 state absorption spectra, Möbius aromatic species showed broad, weak and featureless spectral features with small extinction coefficients in line with typical antiaromatic expanded porphyrins. With the aid of quantum calculations, these results indicate that the Möbius aromatic nature in the S0 state is reversed to Möbius antiaromaticity in the T1 state. This is the first determination of triplet excited state aromaticity with stable Möbius aromatic molecules.

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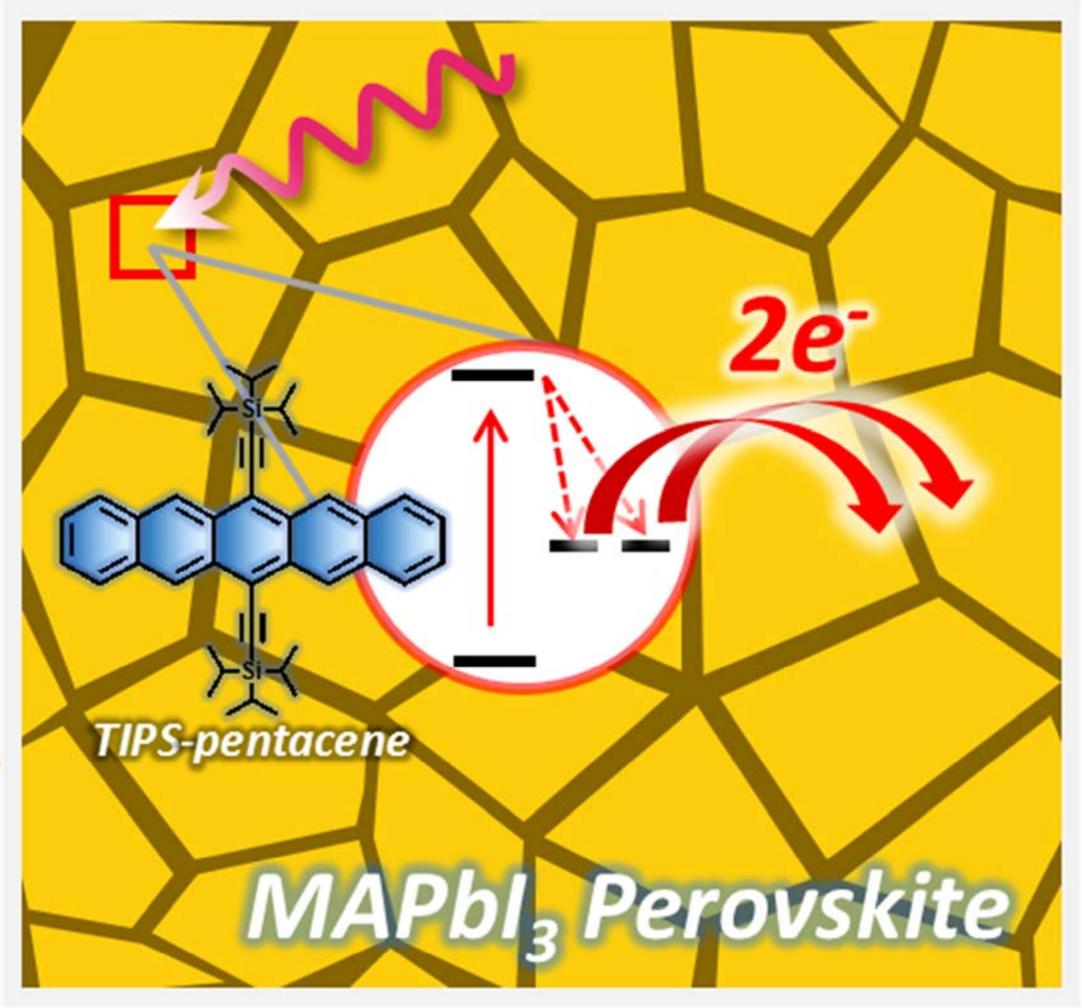
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-70**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electron Transfer from Triplet State of TIPS-Pentacene Generated by Singlet Fission Processes to MAPbI$_3$ Perovskite

이상수 김동호*

연세대학교 화학과

To reveal the applicability of singlet fission processes in perovskite solar cell, we investigated electron transfer from TIPS-pentacene to $CH_3NH_3PbI_3$ (MAPbI$_3$) perovskite in film phase. Through the observation of the shorter fluorescence lifetime in TIPS-pentacene/MAPbI$_3$ perovskite bilayer film (5 ns) compared to pristine MAPbI$_3$ perovskite film (20 ns), we verified electron transfer processes between TIPS-pentacene and MAPbI$_3$ perovskite. Furthermore, the observation of singlet fission processes, a faster decay rate, TIPS-pentacene cations, and the analysis of kinetic profiles of the intensity ratio between 500 and 525 nm in the TA spectra of the TIPS-pentacene/MAPbI$_3$ perovskite bilayer film indicate that electron transfer occurs from triplet state of TIPS-pentacene generated by singlet fission processes to MAPbI$_3$ perovskite conduction band. We believe that our results can provide useful information on the design of solar cells sensitized by singlet fission processes and pave the way for new types of perovskite solar cells.



2e$^-$
TIPS-pentacene
MAPbI$_3$ Perovskite

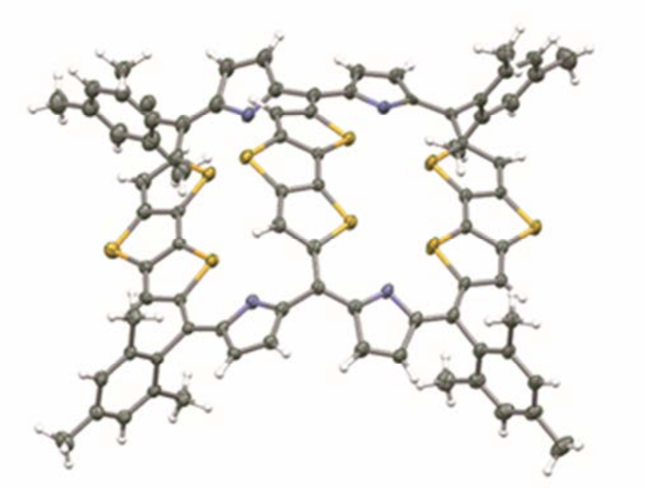
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-71**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Bicyclic Baird-type Aromaticity

차원영 김동호*

연세대학교 화학과

Classic formulations of aromaticity have long been associated with topologically planar conjugated macrocyclic systems. The theoretical possibility of so- called bicycloaromaticity was noted early on. However, it has yet to be demonstrated by experiment in a simple synthetic organic molecule. Here, we detail the synthesis and characterization of two congeneric nonplanar dithienothiophene bridged [34]octaphyrins that permit access to two different aromatic forms as a function of oxidation state. In their neutral forms, these systems contain competing 26 and 34 π-electronic circuits. When subject to two-electron oxidation, electronically mixed [4n+1]/[4n+1] triplet biradical species are obtained that display global aromaticity in accord with Baird's rule.



일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-72**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Time-Resolved fluorescence studies on the Excited State Proton Transfer Reaction of C183 in Aqueous NaCl Solutions

김상인 정준영 박성남*

고려대학교 화학과

Proton transfer is conceptually and practically important in physics, biology, and chemistry. A photoacid has been used as a good molecular system to investigate the proton transfer mechanism in aqueous solutions. In this study, Coumarin 183 (C183), which is a photoacid, was used to study the excited-state proton transfer (ESPT) reaction in aqueous NaCl solutions. When C183 is electronically excited, C183 (ROH) fluorescing at 410 nm undergoes ESPT reaction in which a proton dissociates from C183 producing C183 anion (RO^{-}) which emits fluorescence at 450 nm. Steady-state and time-resolved emission spectroscopy were used to study the kinetic and thermodynamic properties of ESPT reaction of C183 in aqueous NaCl solutions. Steady-state emission spectra show a correlation between the NaCl concentration and the acid dissociation equilibrium constants of C183 on the excited state (ROH* and RO^{-*}). Time-resolved fluorescence signals were measured at several temperatures by using a time-correlated single photon counting (TCSPC) method. The activation energies for the ESPT were determined at different NaCl concentrations. Quantum chemical calculations were performed to optimize the local hydrogen-bonded (H-boned) configurations of C183 in aqueous NaCl solutions. It is found that the activation energy for the ESPT is highly associated with the local H-bond configurations of C183 which significantly influenced by dissolved ions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-73**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Exciton and Polaron Diffusion Processes in Polythiophene Films with Localized Aggregates

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연세대학교 화학과 [1]POSTECH 화학공학과

Photoelectron conversion efficiency in organic solar cells based on π-conjugated polymers is heavily dependent on their complex microstructures. Based on the experimental consensus that polymers films with large crystalline domains often transport excitons and polarons better than amorphous structures, persistent efforts have been put to engineer polycrystalline structures until a number of highly disordered amorphous polymer films with comparable or higher charge mobility recently contradicted such belief. It has been suggested that high charge carrier mobility is a consequence of interchain hopping aided by intrachain through-bond transfer process which permits connectivity between crystalline domains. In order to test the effect of enhanced interdomain connectivity we prepared poly(3-hexylthiophene) films containing a portion of thiophene units without hexyl groups randomly incorporated in polymer chains to form planarized backbone and small localized aggregates. By employing time-correlated single photon counting technique, singlet exciton diffusion processes of the random copolymer and homopolymer in various temperature conditions are analyzed. Continuous wave photomodulation spectroscopy and nanosecond transient absorption spectra will be present to compare the polaron diffusion dynamics of polymer films with two distinctly different microstructures.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-74**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

pyQSAR : fast QSAR modeling method using Clustering and Monte Carlo search

김신영 조광휘*

숭실대학교 생명정보학과

Chemical properties of compounds are closely related to the structure of the chemical compounds. So, it is important to find out the relation between properties and structure. QSAR (Quantitative Structure Activity Relationships) is one of the methods for finding the relationship between property and structure. However, current the QSAR method has many problems. Modeling process using QSAR has many stage. Each stages may need different software or modules. So the data of each task doesn't integrate with each stages. Another problem is that the number of possible combinations of combining descriptors enormous. For example, the number of possible combination of getting 4 descriptors out of 5,000 descriptors is 5,000C4. That point spends lots of time and needs repetitive work. So, we need a new algorithm for searching the optimal combination of descriptors quickly with a high accuracy score of QSAR model. Also we need unified platform that combine each step of QSAR modeling process. PyQSAR support the foregoing points that we have recognized as problems of existing QSAR process. So, users of pyQSAR don't need to move data and memory. They can produce the whole process result for exporting QSAR models. Usually descriptors selection for building QSAR model is required various machine learning algorithm like a genetic algorithm. But pyQSAR use only single algorithm that combined clustering method with Monte Carlo algorithm. Through the that way, pyQSAR can find the optimal combination of descriptors with high accuracy score quickly. Our results of testing pyQSAR shows that performance of pyQSAR is better than established theses.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-75**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoluminescence of $AgIn_5S_8$ nanoparticles in defect emission

정성현 한노수 송재규*

경희대학교 화학과

The emissive relaxation processes of $AgIn_5S_8$ nanoparticles still remained ambiguous, due to the complicated compositions and the nonnegligible density of structural defects. The emission of $AgIn_5S_8$ nanoparticles was investigated by the steady-state and time-resolved photoluminescence (PL) spectroscopy. The predominant emission showed the large Stokes shift and the long lifetimes, suggesting the defect emission of the nanoparticles. In time-resolved PL spectra, the defect emission was deconvoluted by two Gaussian bands. The relative intensities of two bands changed with increasing detection time, indicating that the lifetime of the high-energy emissive component was shorter than that of the low-energy one. The relative contribution of high-energy emissive component decreased with increasing size, which was ascribed to the reduced surface-to-volume ratio of the nanoparticles. It suggested that the higher-energy emissive state was attributed to the surface defects. As a result, the emissive defect states of the $AgIn_5S_8$ nanoparticles exhibited two dominant relaxation processes from the intrinsic and surface states.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-76**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

SERS-based Facile Detection of Glucose in Human Serum

FU CUICUI 진실아 오주희 정영미*

강원대학교 화학과

An ingenious and facile surface-enhanced Raman scattering (SERS) sensor based on the enzyme catalytic reaction and silver ions-mediated amplification effect was designed for the determination of glucose. In this approach, 4-aminothiophenol (4-ATP) molecules assembled on the surface of gold wafer (Au wafer@4-ATP) act as not only Raman tags but also linkage agents. On the other hand, the silver nanoparticles marked with cysteamine (AgNP@cys) were employed as the components of SERS enhancement. We have traced the SERS intensity of 4-ATP to determine the concentration of glucose in phosphate buffer as low as 0.1 mM, and further obtained the lowest detectable concentration of 0.5 mM glucose in human serum, which shows this approach has the potential for practical applications.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-77**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Molecular Orientation of Poly(3-hydroxybutyrate- co-3-hydroxyhexanoate) and Its Blend with Polyethylene Glycol in Thin Films

Yujing Chen Noda Isao[1] 정영미[*]

강원대학교 화학과 [1]Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, USA / Danimer Scientific, Bainbridge, GA 39818, 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 molecular orientation of PHBHx with different HHx content in thin films using grazing-incidence wide-angle X-ray scattering. We found that increasing the HHx content will change the lamellar orientation of pure PHBHx from edge-on lamellar to flat-on lamellar. The thermal behaviors of such densely packed lamellae crystals were examined by temperature-dependent infrared-reflection absorbance spectroscopy and two-dimensional correlation analysis. Detail information will be discussed in the presentation.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-78**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Detection and Identification of Bacteria Based on SERS

진실아 오주희 박연주 정영미*

강원대학교 화학과

Bacteria can be beneficial or harmful to humans depending on the species. Therefore, in order to prevent damages caused by biological weapons, fast and accurate determination and identification of bacteria should be performed. Surface-enhanced Raman scattering (SERS) is a powerful technique to detect biological reagent because it provides rapid and ultrasensitive detection with a large amount of fingerprint information for the identification of biological materials. In this study, silver nanoparticles was used for detection of bacteria and specific SERS dataset was used for identification of bacteria. Details on analysis of bacteria based on SERS will be discussed.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-79**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Detection of nerve agent simulants using SERS active substrate

오주희 진실아 박연주 정영미*

강원대학교 화학과

The countering and preventing terrorism became a big issue, because terrorism risks are continuing globally. Therefore, many researchers have been investigated for quick and effective detection of CBR (chemical, biological, and radiological) materials. Nerve agents are one of the CBR materials to affect the nervous system of the human body which are a kind of phosphorous-containing organic chemicals. It is difficult to detect this material due to its property that can be readily vaporized or aerosolized. Surface-enhanced Raman scattering (SERS) is a sensitive and effective analytical technique for detection of materials. In this study, we fabricated the SERS substrate with hfipbb (4,4'-(Hexafluoroisopropylidene) bis(benzoic acid)) on the self-assembled Ag nanoparticles monolayer for detecting nerve agent simulants. We successfully detected nerve agent simulants using this substrate by SERS. Details on the result of detecting nerve agent simulants using this SERS substrate will be discussed in the presentation.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-80**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and characterization of bismuth oxide and Ytterbium oxide nanoparticles for CT contrast agent

ADIBEHALSADAT GHAZANFARI SEYEDHOSSEIN 이강호*

경북대학교 화학과

Until now there are many metal oxide nanoparticles that were synthesis for CT contrasting agents. In this work we studied two type of nanoparticles that D-glucoronic acid coated Bi_2O_3 and Yb_2O_3 for CT contrast agent, also we synthesized for using in vitro and in vivo. 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 and Ytterbium oxide nanoparticles. All the synthesized metal oxide nanostructures were characterized by transmission electron microscopy, powder X-ray diffraction and IR spectroscopy.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-81**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The study on the real-time monitoring the cathode surface of Li-ion battery

김수민 박유정 박연주 정영미*

강원대학교 화학과

Li-ion batteries are a rechargeable secondary battery and a promising energy storage devices. But, It has difficulty for applications as an energy source due to the loss of electrochemical performance by side reaction from cathode. Therefore, development of suitable technology that monitoring the electrodes during the operation of the battery is of importance for better understanding of the fatigue of the battery and designing of enhanced lithium-ion battery. Using Raman spectroscopy, we investigated the surface change of the LiCoO2 cathode in the battery in real time. We also performed 2D correlation spectroscopy (2DCOS) to identify surface change mechanism of the cathode materials at the molecular level during charging process. Details of the results will be discussed in this presentation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-82**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Size-Dependent Structure of meso-meso Directly Linked Porphyrin Arrays Probed by Single-Molecule Fluorescence Spectroscopy

이상현 김동호*

연세대학교 화학과

The meso-meso directly linked zinc(II) porphyrin arrays are appealing owing to the expected simple rod-like molecular shape and the repeated regular arrangement of porphyrin rings with large electronic interactions. These properties are also interesting in view of a potential use as photonic molecular wire. As the porphyrin array, whose flexibility is determined by the number of porphyrins, has more porphyrin units, it will easily be a bent structure. Also, if the environment of the molecules is crowded, the structures of the arrays are seemingly bent.By using single-molecule excitation polarization fluorescence spectroscopy (ExPFS), we studied the structure of directly linked porphyrin arrays with different size (ZN, N=1, 2… 64, 96, and 128). ExPFS provides information about anisotropy of absorbing dipoles in multichromophoric molecular systems and has typically been used to assess the degree of structural disorder in conjugated polymers. In the measurement of the modulation depth (M), we revealed that porphyrin arrays have bent structure as their size increases, representing the long arrays have bent structures. Detecting the change of M values depending on length shows how many porphyrin units act as an absorbing unit. Our study provides the guidance for the design of molecular system that can enhance the performance of molecular rods.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-83**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dynamic Planarization Process in the excited-state of Cyclic Oligothiophene 12-Mers Modulated by its π-Linkers

김준오 김동호*

연세대학교 화학과

Organic π-conjugated materials have drawn considerable attention in recent years due to their great potential for applications in various optoelectronic devices. Among several approaches to improve the performance of these devices at the molecular level, it has been reported that linkers between functional units play a decisive role in modulating the optical and semiconducting properties, since they can effectively control the rigidity of conjugated backbone [1-3]. However, numerous studies on the linker effects focused only on linear conjugated systems, and there have not been any detailed studies on cyclic counterparts, despite of enormous interest in these materials. In this work, we scrutinized the linker effects in the dynamic planarization processes of a series of π-conjugated cyclic oligothiophene 12-mers, where the number of ethynylene and vinylene linkers was chosen to modulate the rigidity of cyclic backbone. From transient fluorescence spectra obtained using broadband fluorescence up-conversion technique [4], we extracted two valuable parameters, the spectral center of mass (νCOM) and fluorescence intensity ratio between 0-0 and 0-1 vibronic bands (I0-1/I0-0), in order to trace the progress of dynamic planarization processes. With these data, we demonstrate that the vinylene linkers induce faster dynamic planarization processes, higher degree of planarity and longer exciton delocalization length along the cyclic conjugated backbone. Molecular dynamics simulations and density functional theory calculations also greatly support that the vinylene linkers play a key role in making cyclic backbone more planar by reducing torsional disorder, which leads to longer π-conjugation.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-84**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of Pendant Side Chains of π-Linkers on Symmetry Breaking Intramolecular Charge Transfer Dynamics in Centrosymmetric Diketopyrrolopyrrole Derivatives

김우재 김동호*

연세대학교 화학과

The effect of the length of pendant side chains in centrosymmetric quadrupolar molecules on dynamics of their most intriguing photophysical phenomenon, i.e., symmetry-breaking intramolecular charge transfer, has been explored. Unexpectedly, we found that there is a considerable influence of length of pendant side chains in π-linkers arose as a structural factor enabling the control of the degree of fluorescence solvatochromism. The symmetry-breaking intramolecular charge-transfer dynamics has been described on quadrupolar diketopyrrolopyrrole derivatives possessing fluorene moieties as π-linkers and diarylamino groups as electron donors. Based on the evolution of time-resolved fluorescence spectra obtained by a femtosecond broadband fluorescence up-conversion spectroscopy, it was found that the relative contribution of diffusive solvation and torsional relaxation in overall spectral relaxation can be modulated by the length of pendant side chain. Consequently, we demonstrated that this modulation plays a significant role in determining the photophysical properties of diketopyrrolopyrroles in a polar medium.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-85**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

FTIR Study : LiPF6 solvation structure in highly concentrated nonaqueous Electrolytes

김민주 곽경원*

고려대학교 화학과

Lithium ion battery(LIB) is indispensable material in daily life for the portable energy storage devices. For this reason, various studies of LIB have been steadily done specially in the efficiency of this battery. In this investigation, We focus on electrolytes, which is a major component of LIB system, used for transporting Li ion between cathode and anode. There are many researches how electrolytes, in general carbonates, form solvation structure and are involved in the mobility of Li ion. We measure the FTIR spectrum (1) single solvent system of cyclic or acyclic carbonate (2) binary solvent system of mixture of cyclic and acyclic carbonate depending on the concentration of LiPF6, the basic Li ion salt, setting maximum ionic conductivity as a standard that represents the performance of LIB. Through this study of FTIR spectroscopy, We recheck previous researches and find the supporting data about relation of solvation sheath with LIB efficiency.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-86**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Relaxometric and In Vivo MRI Application of Mixed Zn(II)/Gd(III) Oxide Nanoparticles

양병우 이강호*

경북대학교 화학과

The D-glucuronic acid coated Zn(II)/Gd(III) oxide nanoparticles (Zn = ~ 8 mole percent) were synthesized in a polyol method. Non-magnetic Zn(II) ions were mixed into Gd_2O_3 nanoparticles. The nanoparticles were characterized with HRTEM, XRD, FT-IR, TGA, SQUID magnetometer, and MRI instrument. The nanoparticle was estimated to be 2.1 nm. The hydrodynamic diameter was estimated to be 7.3 nm. The surface coated nanoparticles showed $r_1 = 12.3\ s^{-1}mM^{-1}$ ($r_2/r_1 = 1.1$), corresponding to an ideal condition for T_1 MRI contrast agent. We attribute this to reduced magnetization of the mixed nanoparticles. The surface coated nanoparticles were non-toxic from cytotoxicity test. Their effectiveness as a T_1 MRI contrast agent was confirmed by acquiring in vivo T_1 MR images of a mouse after intravenous injection.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-87**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Characterization of polyacrylic acid coated Ultrasmall gadolinium oxide nanoparticles

MiaoXu 이강호*

경북대학교 화학과

The relaxometric properties of ultrasmall Gadolinium oxide ($Gd2_2O_3$) nanoparticles coated with various biomedical applications because of excellent physical properties of Gd(III). Gd(III) has the highest spin magnetic moment of all elements arising from 7-unpaired 4f-electrons suitable for positive (or T1) magnetic resonance imaging (MRI) contrast agents, a high X-ray attenuation coefficient suitable for X-ray computed tomography (CT) contrast agents. In this poster, researchers synthesized gadolinium oxide nanoparticles modified with different size ligands which are synthesised in triethylene glycol as MRI contrast agents. They are characterized with FT-IR, Toxicity test, XRD, TGA, TEM and MRI instrument. Relaxometric properties of Gd_2O_3 nanoparticles coated with these large ligands were studied.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-88**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Gadolinium oxides nanoparticles coated by poly(acrylic acid)-rhodamine as bimodal MRI – cell labeling agents

HOSONLONG 이강호*

경북대학교 화학과

The combination of a magnetic resonance imaging (MRI) agent and a cell labeling (CL) agent can provide high resolution spatial images around cancer cells. In this work, gadolinium oxides nanoparticles which were coated by poly(acrylic acid)-rhodamine showed high T_1 and T_2 relaxivities (T_2:T_1 ≈ 1.3) and low cytotoxicity to cells. Gd_2O_3 NPs were well coated and have small hydrodynamic size which help Gd_2O_3 NPs to be fully excreted from the body through the renal system to avoid any danger such as nephrogenic systemic fibrosis. Due to the presence of rhodamine moiety, Gd_2O_3 NPs also showed fluorescent and pH-responsive property which can be used to differentiate normal and cancer cells *in vitro*.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-89**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Extension of Baird's Rule to Twisted Heteroannulenes:Aromaticity Reversal of Singly-Twisted and Doubly-Twisted Molecular Systemsin the Lowest Triplet State

홍용석 김동호*

연세대학교 화학과

I have investigated the lowest triplet state (T1) aromaticity of singly-twisted Möbius aromatic and doubly-twisted Hückel antiaromatic bis(palladium(ll)) [36]octaphyrins using spectroscopic measurements and quantum calculations. In the T1 state absorption spectrum, singly-twisted Möbius [36]octaphyrin showed broad and weak absorption spectral features, which is analogous to those of antiaromatic expanded porphyrins. On the other hand, the T1 state absorption spectrum of doubly-twisted Hückel [36]octaphyrin exhibited intense and distinct features, representing aromatic nature. The quantum calculations based on magnetic and topological indices support the reversed aromaticity in the T1 state. Furthermore, I have revealed that the degree of structural smoothness affects the aromaticity reversal in the T1 state.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-90**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Influence of π-conjugation structural changes on intramolecular charge transfer and photoinduced electron transfer in donor-π-acceptor dyads

김소연 조대원 강상욱 손호진*

고려대학교 신소재화학과

The influence of π-conjugation structural changes on photoinduced electron transfer (PET) and intramolecular charge transfer (ICT) processes in π-conjugated donor (D)-acceptor (A) dyads (D-π-A) was investigated. Three types of D-π-A dyads were prepared through the modification of the structure of their π-conjugated linker, including D-π-A (1), D-π_{tw}-A (2), and D-π-Si-π-A (3) . In these dyads, cz and ox moieties acted as D and A, respectively. The emission maxima of dyads 1 and 3 red-shifted with the increase in polarity, which could be attributed to the ICT process. The fluorescence lifetimes for dyads 1 and 3 were 2.64 and 4.29 ns, respectively. In contrast, dyad 2 showed dual emission at 350 and 470 nm. The emission of dyad 2 at 380 nm corresponded to the monomer fluorescence in the locally excited state. Moreover, the emission at 470 nm increased with the diminishing of the fluorescence at 380 nm. This emission band can be assigned as the intramolecular exciplex emission, and showed a strong solvatochromic shift. The low emission quantum yield (* state, thus the PHT takes place from $1A^*$ to D through the HOMO levels within few picoseconds. On the other hand, when the donor moiety is excited at 340 nm, the PET process occurs from $1D^*$ to A. Based on fs-TA studies, it was found that the dynamics and mechanisms for the charge transfer were strongly affected by the variation of the π-conjugation of the linker.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-91**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

e-beam-induced Phase Transformation of Gold Nano Sheet from Metastable Hexagonal Close-packed to Face-centered Cubic Structure

민경석 박상원[1] 김성근[2,*]

서울대학교 생물물리 및 화학생물학부 [1]서울대학교 생물물리 및 화학생물학과 [2]서울대학교 화학부

Although gold (Au) is most stable as face-centered cubic (fcc) structure in solid state, hexagonal close-packed (hcp) nano square sheets of Au (AuSS) have recently been synthesized on graphene oxide (GO) sheets under ambient condition. We found in real time that a AuSS with the edge length of 100–600 nm and the thickness of less than 6 nm undergoes a phase transformation from hcp to fcc structure under the e-beam irradiation condition of transmission electron microscope (TEM). We propose a mechanism for the observed phase transformation of metastable AuSS.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-92**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Binding Free Energy Calculation for protein-ligand docking using Clustering and MD simulation

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숭실대학교 생명정보학과

The whole process of commercializing a new drug requires tremendous amount of time and money. For this reason, to improve the successfulness of developing a new drug, it is important to begin the development process with a compound design that has a high success rate of synthesis. By predicting the possibility of failure in advance, we can reduce the time and cost of developing a new drug. One of the most common method used to achieve this goal is protein-ligand docking. This method produces relatively fast result. However, there are too many possible poses to begin with. Also, the energy function used is not always accurate, producing energy values that are different from the actual energy values. One method that produces more accurate result than docking is using the Molecular Dynamics Simulation to predict the binding free energy value. However, using the MD simulation to calculate all the possible ligand poses takes too much time.This research proposes clustering of ligand models to achieve this goal. To solve this problem, we used the clustering method to group ligand poses that are created through the protein-ligand docking, and selected representative poses for each cluster for the purpose of reducing the number of poses to work with. The selected ligands were then applied with the MD simulation to calculate the binding free energy values and compare with the energy values from docking. As a result, we were able to confirm that the clustering and MD simulation produced better result in predicting the best ligand pose compared to docking.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-93**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Distinct mechanisms for the upconversion of NaYF4:Yb3+,Er3+ nanoparticles revealed by stimulated emission depletion

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GIST 화학과 [1]GIST [2]GIST 물리화학부 화학과

Upconverting nanoparticles (UCNPs) have attracted enormous interest in the past few years owing to their unique optical properties and potential for various applications such as bioimaging probes, biosensors, and light-harvesting material for photovoltaics. For the biological applications, the improvement of imaging resolution is one of the most important goals. The super-resolution imaging techniques, which overcome the fundamental diffraction limit of light, rely on the photochemistry of the organic dyes or fluorescent proteins. We hereby report our studies toward super-resolution microscopy with UCNPs. We found that the red emission (655 nm) of core/shell UCNPs (NaYF4:Yb3+,Er3+/NaYF4) could be modulated by emission depletion (ED) of the intermediate state that interacts resonantly with IR beam (1540 nm). On the other hand, the green emission bands (525 and 545 nm) were nearly invariant upon the IR beam irradiation. The origin of such distinct behaviors between the green and red emissions was attributed to their different photophysical pathways.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-94**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Quinophthalone Displays Uncommon N-to-O Excited State Intramolecular Proton Transfer (ESIPT) Between Photobases

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서울대학교 화학부 [1]서울대학교 생물물리 및 화학생물학과 [2]상명대학교 의생명공학과

Excited state dynamics of common yellow dye quinophthalone (QPH) was probed by femtosecond transient absorption spectroscopy. Multi-exponential decay of the excited state and significant change in rate constants upon deuterium substitution indicate that uncommon nitrogen-to-oxygen excited state intramolecular proton transfer (ESIPT) occurs. Unlike most cases of ESIPT, QPH does not exhibit tautomer emission, possibly because of the adiabatic surface crossing between the S_1 and S_2 states, which we verified by the density functional theory (DFT) and time-dependent density functional theory (TDDFT) calculations. The ESIPT of QPH is a highly interesting case also because the moieties participating in ESIPT, quinoline and aromatic carbonyl, are both traditionally regarded as photobases.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-95**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Significantly Improved Chemical Stability of Silver Nanodots via Anchor-Induced Encapsulation in Silica Nanoparticles

양선아 최성문 Junhua Yu*

서울대학교 화학교육과

Single stranded DNA (ssDNA) encapsulated silver nanodots (AgNDs) exhibit not only large molar extinction coefficients, outstanding luminescence quantum yield, but also high emission bright. Although ssDNA encapsulated AgNDs have great potential as biological imaging agents due to their remarkable photo-physical properties, the coordination bonding nature between silver nanodots and their protection groups might be vulnerable to chemical quenching in aqueous solution due to destabilization by competition coordination. Encapsulation of silica nanoparticles have been applied to organic dyes, gold clusters and silver nanoparticle for improvement of their stability in biological application. In this report, we investigated the factors that influence the stability of AgNPs and examined several nanoparticle platforms in order to construct chemically stable product. We found that the chemical stability of silver nanodots was significantly improved via anchor-induced encapsulation in silica nanoparticles while retaining their excellent photophysical properties.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-96**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

One-photon mass-analyzed threshold ionization (MATI) spectroscopy of thietane:Determination of accurate ionization energy and ring-puckering vibrational mode

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강원대학교 화학과 [1]서강대학교 화학과

We have measured the high-resolution vibrational spectra of a thietane(trimethylene sulfide) cation in the gas phase by employing the vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopic technique. Peaks in the low frequency region of the observed MATI spectrum of thietane originate from a progression of the ring-puckering vibrational mode (typical in small heterocyclic molecules), which is successfully reproduced by quantum-chemical calculations with 1D symmetric double-well potentials along the ring puckering coordinates on both the S_0 and D_0 states, the ground electronic states of neutral and cation of thietane, respectively. The values of the interconversion barrier and the ring-puckering angle on the S0 state, the parameters used for the quantum-chemical calculations, were assumed to be 274 cm^{-1} and 26°. The barrier and the angle on the D0 state, however, are found to be 48.0 cm^{-1} and 18.2°, respectively, where such small barrier height and puckering angle for the cation suggest that the conformation of thietane cation on the D0 state should be more planar than that of the thietane neutral.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-97**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Vibrational Solvatochromism Studies of Amide Ⅰ Mode Using the SolEFP method

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고려대학교 화학과

Vibrational solvatochromism is the process of the changes in the vibrational absorption spectrum due to molecular surrounding changes. To study the environment of a molecule, we often use properly chosen chromophores. I will discuss carbonyl IR probe among chromophores. The first consideration in carbonyl IR probe is Amide Ⅰ mode which occurs naturally in proteins and it means the vibrations of the peptide group. Therefore, I want to deal with a system consisting of water and N-Methylacetamide (NMA) which has peptide group. As a result, I obtained frequency shifts using the SolEFP method. In addition, ion (Na+) and NMA systems will be discussed and compared with the previous (water & NMA) system.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-98**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Structure and orientation change according to the various pH conditions of 4-amino-4’-cyanobiphenyl on silver surfaces: SERS and DFT study

엄소영 김홍래* 권찬호*

강원대학교 화학과

Adsorption behavior of 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 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.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-99**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Conformer and stereo-isomer specific vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy of tetrahydrofuran and crotonaldehyde

박성만 김홍래[*] 권찬호[*]

강원대학교 화학과

We measured vibrational spectrum of cationic tetrahydrofuran (THF) and crotonaldehyde (2-butenal) utilizing the one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. From the origin band of VUV-MATI spectrum, adiabatic ionization energy of cationic ground state of THF was determined to be 9.4259 ± 0.0007 eV. This value is agreement with previously value 9.427 eV. Most of observed vibrational peak could be assigned on twisted C_2 symmetry structure through the Franck-Condon simulation. Based on the excellent agreement between the experimental and quantum chemical calculated results, the only twist form of the C_2 symmetry for the cation was determined to be stable. The specifically stereo-isomeric VUV-MATI spectra of crotonaldehyde were measured and analyzed comparing with the Franck-Condon simulations and ionization energies for four stereoisomers of trans-s-cis-, trans-s-trans-, cis-s-trans-, and cis-s-cis- crotonaldehyde calculated at M062x/aug-cc-pVDZ level. First, the ionization energy of trans-s-trans conformer of trans-s-trans-crotonaldehyde was accurately determined to be 9.7501 ± 0.0007 eV, in excellent agreement with previously reported value, 9.75 eV. Further calculations at the higher level are performing for the rigorous vibrational assignment of each stereoisomers of crotonaldehyde.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-100**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of hydrazoic acid

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강원대학교 화학과

We recorded for the first time the vibrational spectrum of hydrazoic acid (HN_3) cation in the electronic ground state by using the vacuum ultraviolet mass-analyzed threshold ionization spectroscopy. The tunable vacuum ultraviolet (VUV) radiation was generated by non-resonant four-wave sum frequency mixing ($\omega_{VUV} = 2\omega_{UV}+\omega_{Vis}$) in Xe and Ar mixture. Quantum calculation and Franck-Condon simulation was carried out to assign the peaks and determine the structure, which is linear or ring. Additionally, the ionization energy of HN_3 was determined to be 86591 ± 10 cm^{-1} (10.736 ± 0.001 eV) from the 0-0 band position in the MATI spectrum.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-101**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Dissociation of Sulfur Oxoacids by Two Water Molecules Studied by Ab Initio and Density Functional Theory Calculations

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We have studied geometries and energies of sulfur oxoacids $H_2S_mO_2$ (m=2-4) and their mono- and di-hydrated clusters by using the density functional theory (M062X) and ab initio theory [SCS-MP2 and CCSD(T)] calculations. From the results compared with previously reported disulfuric acid ($H_2S_2O_7$) case, the gas phase acidity is ordered as $H_2S_2O_2 < H_2S_3O_6 < H_2S_2O_7 < H_2S_4O_6$. All these sulfur oxoacids show dissociated (or deprotonated) geometries with only two water molecules, although the order of dissociated conformer energy is different. $H_2S_3O_6$ has the best molecular flexibility to adopt such an H-bonding network structure, and thereby all the low-lying conformers of $H_2S_3O_6(H_2O)_2$ are dissociated, while the least flexible $H_2S_2O_6$ forms such a structure with high strain, and the dissociation of $H_2S_2O_6(H_2O)_2$ is found from the third lowest conformer. Although the gas phase acidity of $H_2S_4O_6$ is highest in this series, the lowest dissociated conformer and the lowest un-dissociated conformer of $H_2S_4O_6(H_2O)_2$ are very close in energy. This is because forming the H-bonding network structure meets some difficulty due to a large distance between two SO_3 moieties. All the dissociated conformers form a unique H-bonding network structure in which a H_3O moiety is H-bonded to each oxygen atom of two SO_3 moieties and the second water, which is in turn H-bonded to a SO_3 moiety. Spaning over the energetic and geometrical results, the intramolecular H-bonding is the important factor for the order of the gas phase acidity, which may indicate the degree of structural flexibility in this molecular series.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-102**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Study of Photo-degradation of Organic solar cell material with Raman spectroscopy

안규상 이희동 곽경원*

고려대학교 화학과

Organic photovoltaics composed of conducting copolymer and fullerenes have many advantages compare to silicon based solar cell such as low-cost, light-weight, solubility, flexibility etc. Moreover, with consistent efforts, power conversion efficiency of OPVs comes up to 12%, OPV shows promising potential to commercialization. However, there is another obstacle to use OPV in daily basis. Because conducting polymer easily goes degradation process in ambient condition and results in sunlight absorption decrease which drops the device performance. Previously, we investigated the degradation process by using Infra-red spectroscopy to know intermediate structure and find out the degradation process strongly related to backbone conjugation breakage. In this work, to see how backbone conjugation affects more sensitively, we use Raman spectroscopy. Furthermore, we use 3 different wavelength laser to show wavelength dependency of degradation process. I hope our findings provide insight into the degradation mechanism of conjugated copolymer and dedicate to progress in OPV devices

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-103**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Study of wettability of Single-walled Carbon Nanotube film formed on textured Si surface

이종택 이준영 양종회 이휘건*

한양대학교 화학과

Superhydrophobic property of CNTs` surface by a combination of specific geometrical structure and chemical composition has been researched for applications as biosensors, biomedical applications, and composites. Solid surfaces having a water contact angle larger than 150° are usually called superhydrophobic, i.e., extremely difficult to wet. This is also referred to as the lotus effect, from the superhydrophobic leaves of the lotus plant.Single-walled carbon nanotube (SWNT) film formed on textured Si substrate having multiscale structures consisted of nanoscale roughness formed on microscale roughness shows a superhydrophobic property. To investigate the effect on wettability of the SWNT film, an applied voltage treatment have been carried out to SWNT film formed on Si substrates in high vacuum. The reversibility of wettability of the SWNT film formed on textured Si substrate was confirmed through the oxidation procedure using an acid mixture of nitric and sulfuric acid and the reduction procedure using the heating treatment. The effect of treatments on contact angles of the surface of SWNT film was discussed to study wettability of SWNT film on hydrophobicity and hydrophilicity.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-104**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fluorescent carbon nanodots : Synthesis and photoluminescence properties

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대구대학교 화학과 [1]대구대학교 화학응용화학과

Carbon nanodots(CNDs), as a new class of carbon nanomaterials have attracted a great deal of interest since their preparation during the process of electrophoresis of single-walled carbon nanotubes. Because of their outstanding properties such as water solubility, photoluminescence, physiological stability, biocompatibility and low toxicity, they have potential applications in energy and bio-related fields. CNDs can be utilized for the storage and transport of electron in solar cells, OLEDs and the detection of metal ions, DNA assays, proteins etc. Various methods to produce CNDs have been reported such as laser ablation, electrochemical carbonization, solvothermal oxidation and microwave-assisted hydrothermal method. In this work, microwave-assisted method was applied to the synthesis of CNDs and photoluminescence properties of CNDs were investigated. CNDs prepared by this method exhibit higher fluorescence quantum yield. Fluorescence peak shifted to the red with the excitation moved to longer wavelength. Fluorescence of CNDs is also dependent on pH. The fluorescence intensity of CNDs decreased as pH decreased. The average size of CNDs measured by TEM is about 15nm in diameter. Complex formation of CNDs with (E)-2-cyano-3-(5'-(4-(diphenyl amino) phenyl)-2,2'-bithiophen-5-yl) acrylic acid was observed as a new fluorescence band appeared at 580nm. Size distribution of CNDs and photoelectric properties will be further investigated.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-105**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effects of Protonation in meso-Substituted Porphyrins on optical properties and structure

이예진 심상덕*

순천대학교 화학과

Protonation of meso-subsituted porphyrins lead to significant shift in B- and Q-bands. However, the origin of the shifts in absorption bands by protonation still remains in open questions. To delineate the cause of this feature, we have obtained optical and photophysical parameters with four types of tetra-meso-substituted porphyrins with phenyl (PPPP), mesityl (MMMM), pentafluorophenyl (FFFF), and aminophenyl (AAAA) peripherals in freebase and diprotonated forms. In addition, we also calculated the optimized structures and frontier molecular orbitals using DFT methods [B3LYP/6-31G] to investigate the effect of protonation on porphyrin structure. Also, we have obtained NCIS value to correlated the aromaticity and optical spectra. The absorption spectra show that diprotonated porphyrins with less bulky peripherals (PPPP and AAAA) show bathochromic shifts in both B- and Q bands by protonation. On the other hand, in the case of porphyrins with bulky methyl or fluorine at the ortho positon of the phenyl groups, Q(0,0) band is blue-shifted while the B band is red-shifted.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-106**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photoexcitation dynamics of S-nitrosothiols

윤호정 임만호* 박성철

부산대학교 화학과

Nitrogen monoxide (NO) is an important regulatory molecule in physiological functions such as vasodilation, neuronal transmission, and platelet inhibition. S-nitrosothiol (RSNO) compounds play a key role in the uptake, intracellular trafficking, and release of NO in biological systems. Most of RSNO molecules are unstable and the tertiary (the number of substituents on the α carbon of the S-NO) RSNO is believed to be more stable than the primary one. However, some of the primary RSNO are very stable. These are S-nitrosoglutathione (GSNO), 2-(nitrososulfanyl)ethanol (ESNO), S-nitrosocaptopril (SNOcap) and S-nitroso-N-acetylcysteine (NACNO). Using femtosecond IR spectroscopy, we have found that the stretching mode of NO in RSNO appears near 1500 cm-1 and a transient absorption appears around 1800 cm-1 when the molecules is excited by a UV photon. The new absorption arises from the NO mode of RSNO in the intermediate electronic state. S-nitroso-N-acetylcysteine (NACNO) and S-nitroso-N-acetylpenicillamine (SNAP) are almost the same except the substitution degree. Comparative study of NACNO and SNAP will be carried out to understand the relationship between the stability of RSNO and the degree of the substitution as well as the role of the intermediate electronic state of RSNO.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-107**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Computational Study on Vibrational Spectral shift in different size of Water Clusters

임종현 남연식 **FRANCIS KIRBY BURNEA** 이진용*

성균관대학교 화학과

The vibrational Stark effect (VSE) is shift of vibrational spectra induced by an electric field. The VSE is highlighted because it is applied to application and fundamental field. But origin of VSE is still unknown in molecular level. So to understand the origin of VSE, we studied hydroxyl stretching of water clusters. We calculated the Stark tuning rate ($\Delta\mu$), and divided this value into two parts regarding origin of VSE, which are change of nucleic and electronic structure. And we defined the parts as geometric effect ($\Delta\mu_{geom}$) and polarization effect ($\Delta\mu_{pol}$). Using this method, we studied on shape effect, local field effect, and anharmonic effect. For study on shape effect, we considered all O-H bonds in system and calculated both of $\Delta\mu_{geom}$ and $\Delta\mu_{pol}$ respectively. From this method, calculated results show that if bond length of bond varies under a field, $\Delta\mu_{geom}$ is dominant origin of VSE. In other side, $\Delta\mu_{pol}$ is related with rearrangement of electrons. At that time the amount of rearrangement has relevance to present of hydrogen bond. As a result, we found that present of hydrogen bond is important variable. Secondly, about study on local field effect, we compared $\Delta\mu$ under only external field and total field. We also separated local field effect into geometric and polarization local field effects. According to results of the comparison, $\Delta\mu$ is factor determining which local field effect is dominant among geometric and polarization local field effects. At last about anharmonic effect, we investigated variation of bond dissociation energy under a field. As a results, increase and decrease of dissociation energy caused by electric field make anharmonic effect in positive and negative direction, respectively.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-108**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Probing the photophysical properties of *mer*- and *fac*-isomers for tris-cyclometalated homoleptic iridium (III) complexes

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고려대학교 신소재화학과

Two isomeric N-heterocyclic carbene Ir(III) complexes, *f*-Ir-$(dbfmi)_3$ and *m*-Ir-$(dbfmi)_3$, were isolated and their systematic investigation on photophysical and electrochemical properties was carried out. Among them, the crystal structure of the meridional isomer, *m*-Ir-$(dbfmi)_3$, is determined. The origin of phosphorescent emissions differs depending on the configurations of the two isomers. Both isomers, *f*-Ir-$(dbfmi)_3$ and *m*-Ir-$(dbfmi)_3$, showed efficient emission in dichloromethane solution with quantum yields of 68% and 53%, respectively, due to unusual properties of the N-heterocyclic carbene (NHC) ligand; –that is, the complexes possess a strong metal–ligand bond that destabilizes the nonradiative metal centred ligand-field states. Depending on their configurations, the two isomers showed slightly different excited states. Even though both isomers possess a largely ^{3}LC character mixed with the ^{3}MLCT character in their excited states, *m*-Ir-$(dbfmi)_3$ showed higher ^{3}MLCT character as evidenced by the solvent polarity dependence emission spectra and emission lifetime. DFT calculations clearly support this different photophysical property.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-109**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Computational Study of Benzodithiophene Based Derivatives as Hole Transport Material for Perovskite Solar Cell

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Various studies have been dedicated to the development of perovskite solar cell (PeSC) which has a high certified power conversion efficiency of 22.1%. Discovery of a cheaper and more efficient hole transport material (HTM) for PeSC have been an active area of research. Recently, PeSC with sulfur based HTMs have garnered better efficiency compared to the reference device. In this presentation, we designed sulfur-containing benzothiophene central core derivatives as potential HTM for PeSC. Energy levels, absorption spectra and electrochemical properties of the derivatives were investigated using the density functional theory and time-dependent density functional theory.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-110**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Systematically Designed Dye Sensitizers for Solar Cell Applications

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Computational chemistry has been very valuable in the field of solar energy harvesting. In dye-sensitized solar cell (DSSC) for instance, a strategic approach is the molecular engineering of dye sensitizer using reliable and inexpensive computational methods prior to the synthesis of the dyes. In the research presented herein, a series of metal-free dyes were systematically designed for possible applications in dye-sensitized solar cells. We focused in the modification of the π-bridge with the intention of attaining a more effective conjugation along the dye backbone for efficient charge transfer processes. Density functional theory (DFT) and Time-dependent DFT methodologies were employed to investigate the key properties of the dye sensitizers that are necessary to properly understand the primary role of the dyes in the photon-to-electricity conversion in a solar cell device. The geometry, oxidation potential, the electronic structure, and absorption spectra were calculated to fully comprehend the performance of each dye. Also, dye-TiO2 complexes were theoretically optimized to understand the dye-to-semiconductor charge transfer mechanism. These theoretical results may serve as a potential reference for the future dye designs for DSSC applications.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-111**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of surface modification of TiO_2 on photo-catalytic performance by vacuum annealing after PDMS deposition

차병준 우태균 한상욱 김일희 김호종 박찬흠 정재환 서현욱[1] 김영독*

성균관대학교 화학과 [1]상명대학교 화학에너지공학과

The surface of TiO_2 was modified by deposition of polydimethylsiloxane (PDMS) at various temperatures (150, 180, 200, and 250 ^oC) followed by a vacuum annealing process at 800 ^oC. Properties of surface-modified TiO_2 were studied by means of FT-IR, UV-Vis diffuse reflectance, and X-ray photoelectron spectroscopy. We have studied the impacts of surface modification on photo-catalytic activity of TiO_2 by evaluating the photo-catalytic removal of methylene blue (MB) from aqueous solution under UV light irradiation. PDMS coating and a subsequent vacuum annealing resulted in the hydrophilic modification of TiO_2 surface and it resulted in enhanced photo-catalytic activity of TiO_2 compared to bare TiO_2. However, the photo-catalytic activity of surface-modified TiO_2 decreased as the the temperature of PDMS deposition increased. Higher temperature of PDMS deposition resulted in the formation of thicker PDMS films on TiO_2 surface and we evidenced that it can have both the positive and negative influence on the photo-catalytic activity of underlying TiO_2. On one hand, thicker PDMS films produced higher amounts of hydrophilic functional groups by the oxidation of the C-H bonding and PDMS framework (Si-O-Si) after the subsequent vacuum annealing process, which can enhance the photo-catalytic activity. On the other hand, oxidized PDMS framework can act as an insulating layer inhibiting the diffusion of electron-hole pairs from the underlying TiO_2 to the top surface. This negative impact on photo-catalytic activity is much more dominant as the thickness of PDMS layer increased.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-112**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Promoting photo Charge Carrier separation and transportation in CdS by Integrating hetrostructured WS2-MoS2 ultrathin nanosheets for Efficient Solar driven Hydrogen production

devulapalliamaranathareddy 박한빛 마로리 홍상엽 **DHARANI PRAVEEN KUMAR** 김태규*

부산대학교 화학과

Solar-driven photocatalytic hydrogen evolution is important for bringing solar energy–to–fuel energy conversion processes to reality. However, the lack of highly efficient, stable, and non-precious photocatalysts or catalysts designed completely with expensive noble metals have remained elusive, which hampers their large-scale industrial application. Herein, for the first time we designed a highly efficient and stable noble metal-free CdS/WS2-MoS2 nanocomposite through a facile hydrothermal approach. When assessed as a photocatalyst for water splitting, the as-synthesized CdS/WS2-MoS2 nanostructures exhibited remarkable photocatalytic hydrogen evolution performance and impressive durability. We achieved an excellent hydrogen evolution rate of 209.79 mmol•g–1•h–1 under simulated sunlight irradiation, which is higher than those of CdS/MoS2 (123.31 mmol•g–1•h–1) and CdS/WS2 (169.82 mmol•g–1•h–1) nanostructures, and the expensive CdS/Pt benchmark catalyst (34.98 mmol•g–1•h–1). The apparent quantum yield reached 51.4% at 425 nm in 5 h. Furthermore, the obtained hydrogen evolution rate is better than those of several noble metal-free catalysts reported earlier. The observed high rate of hydrogen evolution and remarkable stability may be due to the ultrafast separation of photo-charge carriers and transportation between the CdS nanorods and the WS2-MoS2 nanosheets, thus increasing the number of electrons involved in hydrogen production. We believe that the proposed designed strategy will may open a new door to design advanced noble metal free photocatalytic materials for efficient solar driven hydrogen production.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-113**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

은 나노 입자를 도입한 수산화인회석(Hydroxyapatite)의 향균 작용 연구

표은지

경상대학교 화학과

염기 조건(10 M NaOH)에서 수열합성법을 이용하여 수산화인회석을 합성하였다. 수산화인회석의 표면에 세 가지 서로 다른 농도 (0.1 M, 0.05 M, 0.01 M)에서 이온 교환 반응을 통하여 은을 도입해주었으며, 수소 (4 %) 및 아르곤 (96 %) 기류에서 가열 (200 ℃)하여 은 나노 입자를 생성시켰다. 은이 도입된 수산화인회석(AgHAP) 복합체의 XRD (X-ray diffraction spectroscopy) 실험을 통해 수소 열처리 전에는 2 Theta 값이 33.8°, 36.66°에서 강한 회절이 일어났으며 이는 Ag_3PO_4 가 수산화인회석 표면에 존재한다는 것을 의미하고, 수소 열 처리 후에는 2 Theta 값이 38.2°, 44.4°, 77.6°에서 강한 회절이 일어났으며 이는 Ag 결정이 존재한다는 것을 의미한다. TEM (Transmission Electron Microscope) 실험을 통해서 수소 열처리 전에는 은 나노 입자를 확인 할 수 없었지만, 수소 열처리 후에는 약 4-8 nm 의 은 나노 입자가 생성된 것을 확인했다. AgHAP 의 향균 작용을 조사해본 결과 순수한 HAP 에 비해서 0.1 M 로 이온교환 반응 시킨 AgHAP 가 대략 60 % 향균 억제 효과를 나타내었다. 그러므로 본 연구에서 사용한 은이 도입된 수산화인회석은 향균 작용을 지니는 골 대체제 물질로 사용될 수 있을 것이라 기대된다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-114**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

루테늄을 도입시킨 티타늄 나노시트의 촉매활성 연구

이윤희

경상대학교 화학과

본 연구에서는 특정 농도의 염기조건 (1.67 M NaOH)에서 수열합성법 (hydrothermal method)을 이용하여 티타늄 나노시트를 합성하였다. 합성한 티타늄 나노시트를 RuCl3 수용액에서 UV 조사 및 교반을 함으로써 루테늄을 티타늄 나노시트의 표면에 도입하였다.합성한 루테늄이 도입된 티타늄 나노시트를 산소를 산화제로 이용한 알코올 산화반응에 응용하였다. 특히, 루테늄이 7% 도입된 티타늄 나노시트는 105℃ 1 기압 상에서 벤질 알코올을 다른 부산물 없이 벤즈알데하이드로 86% 산화 되게 하는 촉매활성을 보였다.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-115**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Aromaticity change upon chemical reduction of pentabenzotriazasmaragdyrin

구윤희 김동호*

연세대학교 화학과

Photophysical properties of pentabenzotriazasmaragdyrin (PBTAS), the first example of antiaromatic expanded phthalocyanine and its dianion were examined. Upon chemical reduction using cobaltocene as reductant, we could generate dianion of PBTAS, which exhibits distinctive B-like and Q-like band of aromatic porphyrinoid. Femtosecond transient absorption spectra were examined for both PBTAS and its dianion, yielding characteristic spectral features of antiaromatic and aromatic porphyrinoids, respectively. Quantum chemical calculation conducted on PBTAS and its dianion also reproduces structural and magnetic characteristics of antiaromatic and aromatic species. From these results, we could confirm that chemical reduction on PBTAS results change in its aromaticity from antiaromatic to aromatic.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-116**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Non-stoichiometric $MAPbBr_3$ perovskite and its highly efficient light-emitting diodes

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We report a novel method to prepare highly luminescent $MAPbBr_3$ ($MA = CH_3NH_3$) thin films with in-situ formed nanocrystals based on non-stoichiometric adduct approaches. Excess MABr with respect to $PbBr_2$ in precursor solution plays a critical role as a scaffold which inhibits crystal growth of $MAPbBr_3$, thereby forming nanocrystals. Vacuum-drying process was developed to preserve nanocrystals in the film, which shows a fast radiative lifetime of 3.9 ns along with negligible trapping processes. Based on highly luminescent nanocrystalline MAPbBr3 thin film, efficient green LED with a maximum external quantum efficiency of 8.21% and a current efficiency of 34.46 cd/A was demonstrated.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-117**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Degrees of freedom allowed in the construction of diabatic states: Different diabatization can generate the same results

안희선 백경구*

강릉원주대학교 화학과

The inclusion of nonadiabatic coupling (NAC) effects between nearby electronic states is indispensable in the studies of all photo-physical, photo-chemical, and photo-biological processes. The construction of diabatic states is one of the best ways to handle the effects of NAC and to provide most intuitive understandings. The exact diabatic state, however, cannot be uniquely defined in actual polyatomic systems [1], and many approaches for the construction of near exact semidiabatic state were proposed and used so far. In this work, the degrees of freedom allowed in the construction schemes for diabatic states are analyzed with special emphases placed on three different approaches for H_2S: the earliest scheme [2], the delocalized and regularized diabatization scheme [3] and our recent localized scheme [4]. It will be shown that the three different diabatization schemes all generate the same results. On the basis of the present results and with several theoretical considerations, some new approaches were tested on the ideal model for the isolated conical intersection [5], and possible directions for more practical and straightforward scheme will be discussed. The possibility to accomplish a generalized local diabatization with self-correcting (or self-adjusting) capability will be discussed too.

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장소: 일산 KINTEX
발표코드: **PHYS.P-118**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of substituent position on excimer formation in planar Pt(II) complexes

조양진 김소연 손호진 조대원 강상욱*

고려대학교 신소재화학과

In order to understand the steric influence on excimer formation in square planar metal complexes, three different Pt(II) complexes were prepared by modifying the substituents in the main ligand: Pt-1; the bulky triphenyl silyl (Ph_3Si–) group was substituted at the pyridine moiety (Pt-2) and at the phenyl moiety (Pt-3) of the main ligand of Pt-1. The Pt-complexes showed sky-blue emission at ～460 nm. In addition, Pt-1 and Pt-3 showed excimer emission at ～600 nm in the concentrated solution and the solid sample. The emission lifetimes and intensities for monomeric Pt-1 and Pt-3 showed strong concentration dependence. Indeed, the lifetime of the monomer was reduced in highly concentrated solutions due to excimer formation. The intrinsic emission lifetimes were determined as 364 ns (Pt-1) and 300 ns (Pt-3) by Stern–Volmer analysis, considering the self-quenched lifetime of monomer emission. Pt-2 did not show any excimer emission in the concentrated solution or solid sample. The crystal structures of Pt-1 and Pt-3 were analysed by X-ray crystallographic measurements. The results revealed that the LUMO moiety closely overlapped with that of another Pt-complex. We concluded that the LUMO–LUMO interaction between the pyridine moieties of the main ligand is the main factor responsible for excimer formation.

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장소: 일산 KINTEX
발표코드: **PHYS.P-119**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly Uniform and Monodisperse Gd2O3:Tb3+ Nanoparticles: Synthesis and Characterization

SHANTI MARASINI 이강호*

경북대학교 화학과

Dual mode lanthanide doped gadolinium oxide nanoparticles, which exhibit an excellent magnetic and fluorescence property, have attracted a tremendous attention in the field of biotechnology and nanomedicine. In the present study ultrasmall gadolinium oxide nanoparticles doped with terbium ions were successfully synthesized through polyol method. X-ray diffraction (XRD) result demonstrates that all diffraction peaks are well indexed with the pure cubic shaped Gd2O3. Surface coating was confirmed from Fourier transform infrared (FT-IR) and Thermogravimetric analysis (TGA). Terbium ion significantly influenced the fluorescence property of the particles. The in vitro cytotoxicity of D-glucuronic acid coated Gd2O3: Tb3+ nanoparticles was measured using DU145 and NCTC1469 cell lines and found that nanoparticles are nontoxic up to 200 µM, which is sufficient to use for in vivo MRI imaging.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-120**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

How Deep Is Water Surface?

RashidMdAlMamunur 최철호[1,*]

경북대학교 일반대학원 화학과 [1]경북대학교 화학과

Water surface is an important subject of research in many scientific disciplines and technologies. Despite extensive studies to understand the properties of water surface at a molecular level, the water surface properties still remain many mysteries and controversies especially the origin of the surface charge of water as well as the thickness of surface phase. In order to address the controversies on the surface states of water, we have performed a series of quantum mechanical (QM) molecular dynamics (MD) simulations with advanced water models with and without excess hydroniums and hydroxides. Specific questions explored in this work include the propensities of hydronium ions and hydroxide ions for water surface, the origins of surface charge, their depth distributions and dynamic properties, the orientation of water dipoles, and their contribution to the surface potential and charge.

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발표코드: **PHYS.P-121**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Rotation Barrier of Metastable Isomers of Dodecahedron C20

조용재 이기학[1,*]

원광대학교 바이오나노화학부 [1]원광대학교 화학과, 나노과학기술연구소

Investigate the rotation barrier pattern of dodecaheron C20 carbonStaggered form is more stable than eclipsed formFind Metastable Isomers of Dodecahedron C20 by using QST2

Rotation Barrier of Metastable Isomers of Dodecahedron C_{20}

Yong Jae Cho, Kee Hag Lee,*

Department of Chemistry, and Nanoscale Science and Technology Institute,
Wonkwang University, Iksan, Jeonbuk 54538

Motive

- Investigate the rotation barrier pattern of dodecaheron C_{20} carbon
- Staggered form is more stable than eclipsed form
- Find Metastable Isomers of Dodecahedron C_{20} by using QST2

Method

- Hybrid Density Functional Theory (B3LYP) method with 6-31g(d,p) basic set in Gaussian 03W package

- Using QST2 method with results in Gaussian 03W package

Reference

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3) Lin F; Sørensen E.S.;Kallin C; Berlinsky A.J Handbook of Nanophysics : clusters and fullerene 29, 1-11, 2009

Results

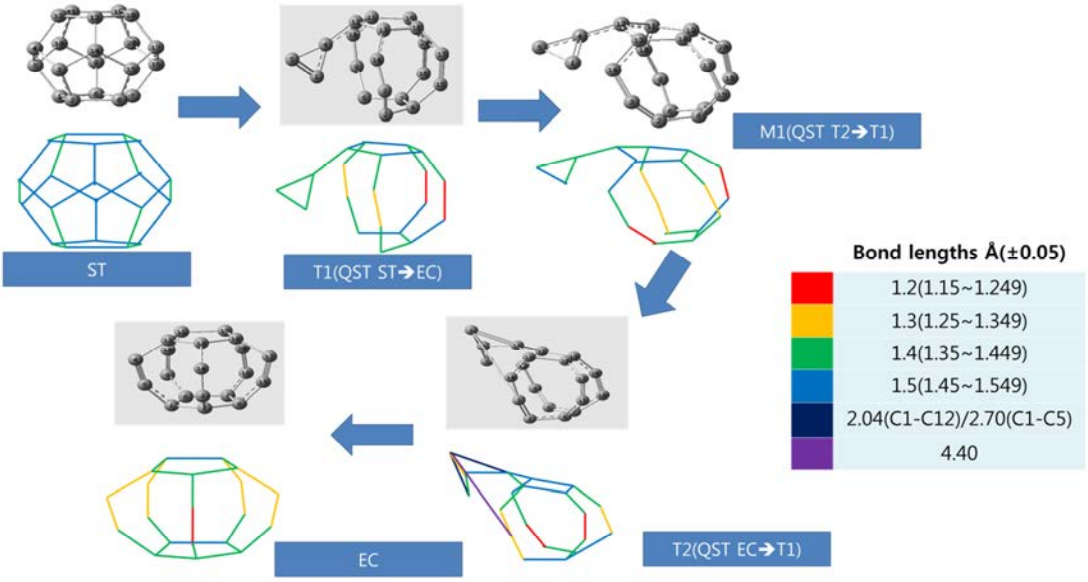

Figure1. Optimized structure of the Metastable Isomers of dodecahedron C_{20} carbon and bond length

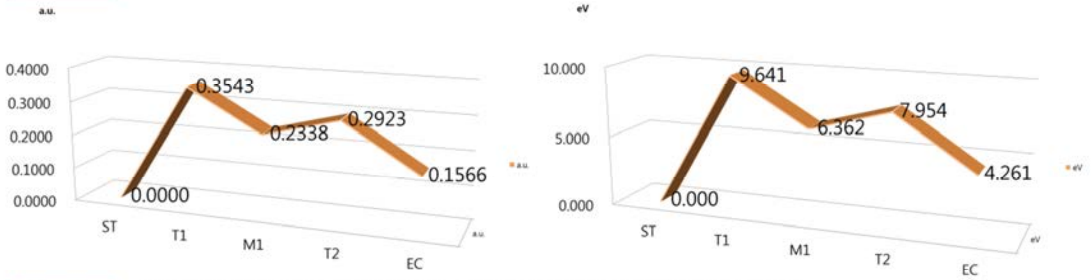

Figure2. B3LYP/6-31g(d) graph au(+761.4443[Ref. E(ST)]=-761.4443) & eV(+20720.111[Ref. E(ST)=-20720.111])

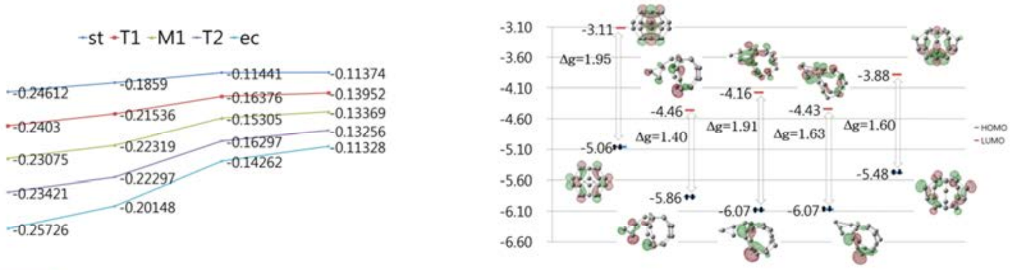

Figure3. The Homo-Lumo Energy

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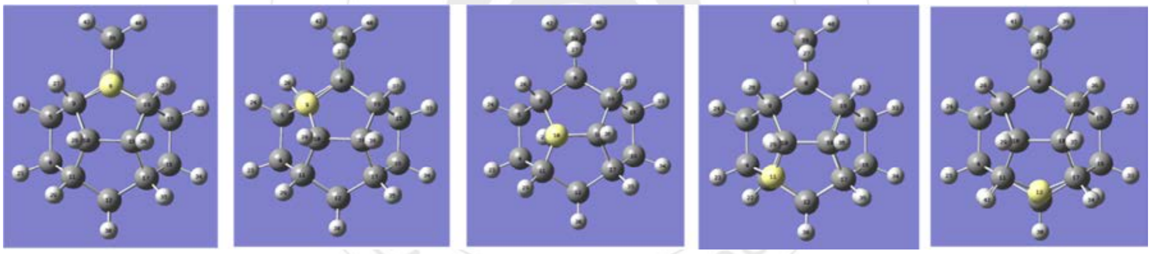
발표코드: **PHYS.P-122**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

spin multiplicity effect of methyldodecahedrane anion by using the hybrid DFT methods

조용재 이기학[1,*] <u>최윤영</u>

원광대학교 바이오나노화학부 [1]원광대학교 화학과, 나노과학기술연구소

spin multiplicity effect of methyldodecahedrane anion by using the hybrid DFT methods



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발표코드: **PHYS.P-123**

발표분야: 물리화학

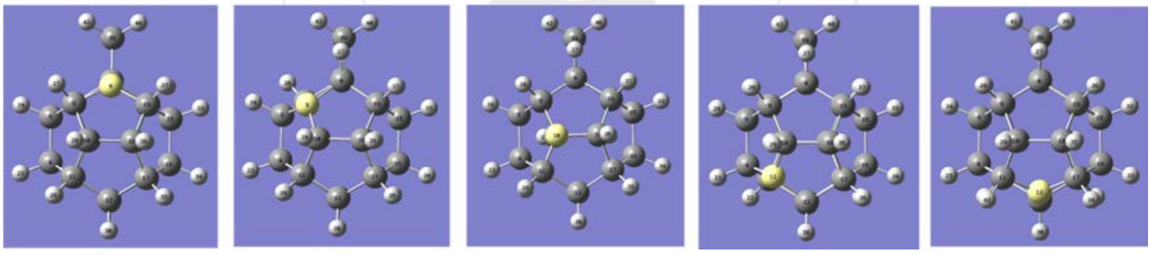
발표종류: 포스터, 발표일시: 목 11:00~12:30

Energy diffrence of methyl dodecahedrane cation isomers by suing the hybrid DFT

조용재 이기학[1,*] 최윤영

원광대학교 바이오나노화학부 [1]원광대학교 화학과, 나노과학기술연구소

Energy diffrence of methyl dodecahedrane cation isomers by suing the hybrid DFT 에너지차 A.U.state(-812.64405)eVstate(-22113.1822)cation-C8-812.64405 0.00000 -22113.18220.0000 cation-C9-812.64328 0.00077 -22113.16150.0207 cation-C10-812.64201 0.00204 -22113.12680.0554 cation-C11-812.64174 0.00231 -22113.11960.0626 cation-C12-812.64181 0.00224 -22113.12120.0610



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장소: 일산 KINTEX
발표코드: **PHYS.P-124**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effects of Boronyl Ligand Manipulation to Dianion: $B_{12}(BO)_{12}^{2-}$

백희현 문지원 김중한*

가톨릭대학교 화학과

The generation of dianions in the gas phase is a difficult task because of the considerable repulsion caused by excessive negative charge. Here, the generation of a very stable dianion ($B_{12}(BO)_{12}^{2-}$) in the gas phase is accomplished by substituting H for boronyl (BO) in a typical dianion, $B_{12}H_{12}^{2-}$. The binding energy of the second electron of the $B_{12}(BO)_{12}$ dianion is 5.99 eV, which represents its stability and is the largest value to date. We clarify that the high stability of $B_{12}(BO)_{12}^{2-}$ originates from the weak π interaction character of the BO ligand. All calculated results indicate the deficient π interaction ability of BO. In addition, $B_{12}(BO)_{12}^{2-}$ is potentially a good candidate for halogen-free electrolytes in Li-ion batteries, as indicated by its Li^+ binding energy being smaller than those of currently used electrolytes.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-125**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Theoretical investigation on the reaction of boron with silane

문지원 백희현 김중한*

가톨릭대학교 화학과

The density functional theory and high-level ab initio calculations were performed to elucidate the detailed reaction mechanism of B + SiH_4 to form the two H atoms bridged structure ($Si(\mu\text{–}H_2)BH_2$). This reaction includes both the thermal and photochemical reactions. On the basis of the calculated results, we propose two subsequent conical intersections where play a crucial role in the photochemical reaction. All calculated results are consistent with the experimentally observed result.

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장소: 일산 KINTEX
발표코드: **PHYS.P-126**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Multifaceted surface adsorption of organic nitriles investigated by SERS

여주현 방윤수[1,*]

GIST 화학과 [1]GIST 물리화학부

Spectral features of the surface enhanced Raman (SER) signal such as vibrational frequencies and bandwidths of vibrational normal modes provide detailed information on the surface adsorption geometry of a molecule on the metal surfaces. In this research, silver colloidal nanoparticles and silver island films were used to obtain SER spectra of -cyano-4-hydroxycinnamic acid (CHCA) and to explain versatile surface adsorption phenomena of organic nitriles. In silver colloidal nanosurfaces, neutral CHCA shows a flat orientation while the surface adsorption occurs via the benzene ring system. As solution pH increases, CHCA deprotonates and both carboxylate and nitrile group of CHCA become main adsorption groups while posing a more or less tilted geometry to the surface. Similar spectral features in the SERS of CHCA have also been with the silver island substrates and the frequency shifts and bandwidth changes in the ν(C≡N) bands in the SERS play a key role in determining the surface adsorption of CHCA. The ν(C≡N) appeared as two split bands; one red-shifted and much broadened might represent the nitrile group which adsorbs mainly on the silver surface via π-electrons of C≡N bond (side-on coordination), the other often with blue-shifts in frequency and band-broadening might represent one which adsorbs on the surface via the nonbonding electron of nitrogen atom (end-on coordination). These adsorption geometry of CHCA can be shown to be widely applicable to other organic nitriles and dinitrile compounds.

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장소: 일산 KINTEX
발표코드: **PHYS.P-127**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Excited-state dynamics of DCM studied by time-resolved electronic and vibrational spectroscopy

이세복 전명삼[1] 전국남[2] 방윤수*

GIST 물리화학부 [1]GIST 물리화학부 화학과 [2]GIST 화학과

4-Dicyanomethylene-2-methyl-6-p-dimethylaminostryryl-4H-pyran (DCM) forms the intramolecular charge transfer between the dimethyl amino (electron donating) group and cyanomethylene (electron accepting) group in the excited states. The charge transfer states of DCM and related push-pull type dyes have been observed in several polar solvents and the structural changes of DCM are proposed to occur in the charge transfer process. However, these structural changes in DCM during the charge transfer reaction in the excited state have scarcely been reported experimentally by time-resolved vibrational spectroscopy.In this work, the details of the charge transfer process upon photo-excitation of DCM will be explored by transient absorption spectroscopy and femtosecond stimulated Raman spectroscopy. The formation and relaxation kinetics of the charge transfer states of DCM in DMSO are measured as 1.5 and 5.9 ps, respectively, by femtosecond transient spectroscopy and another decay lifetime of 1.3 ns is also observed. More importantly, a number of transient Raman vibrational modes including ν(C≡N), ν(C=C) and/or ν(C-C), and δ(CH3) with the charge transfer formation and relaxation dynamics have been observed and will be used to explain the transient structural changes of DCM in the charge transfer state.

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장소: 일산 KINTEX
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발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facilitated Protein-DNA binding with Monte Carlo simulation : controlling distance and scale

정준명 황준필 김태준 김효준*

동아대학교 화학과

We study the combination of three-dimensional diffusive movements and one-dimensional sliding diffusive movements. We research various interval and scale of protein and DNA with simplified facilitated model. We simulate a method that provide numerical exact result. We confirm the results with lattice-based Monte Carlo simulations.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표코드: **PHYS.P-129**
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Tracking the Conformation-dependent Photodissociation Dynamics of $C_2F_4I_2$ in Solution

박성철 박영상 임만호*

부산대학교 화학과

Photodissociation dynamics of C2F4I2 dissolved in CCl4 or acetonitrile was investigated by time-resolved infrared spectroscopy. C2F4I2 in solution has two conformations (anti and gauche) with 80% in the anti-form. When excited with a 267-nm photon, one I atom dissociated immediately (< 0.2 ps), producing two radical forms, anti-C2F4I and gauche-C2F4I. Each radical shows characteristic C−F stretching frequencies: 1321 and 1172 cm−1 for anti-C2F4I and 1272 and 1118 cm−1 for gauche-C2F4I. These frequencies were confirmed by DFT calculation (B3LYP/ cc-pVTZ for C and F, cc-pVTZ-PP for I). The anti-C2F4I in CCl4 undergoes secondary dissociation with a time constant of 180 ps and the gauche-C2F4I with a time constant of 8 ns. When the radical was dissolved in acetonitrile, the anti-C2F4I has a faster secondary dissociation time of 40 ps and the gauche-C2F4I with a time constant of 5 ns. The slower dissociation time can be the dissociation time of the gauche-form or the rotation time from gauche to anti-form. Molecular origin for the conformation-dependent as well as the solvent-dependent photodissociation dynamics will be presented.

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장소: 일산 KINTEX
발표코드: **PHYS.P-130**
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Lattice-based Monte Carlo and Brownian Dynamic Compared to Simulation

황준필 김태준 김효준*

동아대학교 화학과

Monte Carlo simulationMonte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. Their essential idea is using randomness to solve problems that might be deterministic in principle. They are often used in physical and mathematical problems and are most useful when it is difficult or impossible to use other approaches. Monte Carlo methods are mainly used in three distinct problem classes optimization, numerical integration, and generating draws from a probability distribution.I compared two reactions above were confirmed experimentally the differences and the advantages and disadvantages were compared.Brownian Dynamic motionThe collision surface is constantly liquid molecules of an object in liquid. Impact of such liquid molecules is irregular and uneven, but if the surface of the object to the statistical equalization wide. Therefore it does not move any more the size of a large object reaches the mechanical equilibrium in the liquid. However, in micrometers of the fine particles has approximately unit increases the variation in the impact surface is reduced, thereby the movement of the object is irregular in its effects.Diffusion-Influenced Reaction Study on the Compared Efficiency for the Lattice and Brownian MotionsMany 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 presentation, 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.

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장소: 일산 KINTEX

발표코드: **PHYS.P-131**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Determining molecular conformations of heterocyclic molecules by theoretical analysis of VUV/MATI spectra: Solving 1 dimensional Schrödinger equations of a ring-puckering vibrational mode

박정빈 이유란[1] 권찬호[1,*] 김홍래[1,*] 성봉준[*]

서강대학교 화학과 [1]강원대학교 화학과

In nature, small heterocyclic molecules play a role as a reactant in many biochemical reactions and compose other complex compounds. And their activities strongly depend on their molecular conformations. In this respect, identifying the conformations of such molecules by interpreting vibrational spectra is an important work. However, measuring and understanding the vibrational spectrum of heterocyclic molecules with ring-puckering mode, which is the most common vibrational mode of ring-shaped molecule, should be a challenging task. Due to a symmetry in this mode, the degenerate vibrational states appear near the minimum of potential energy surface (PES). On the other hand, near the top of the potential energy barrier, the degenerate states should be splitted with a small energy difference. In experiments, it is hard to observe such a small energy splitting. And even in theory, one should consider the symmetry of the PES to predict (or reproduce) the vibrational spectrum. Therefore, we develop a 1D quantum calculation method that considers the ring-puckering mode and its symmetry. We use trigonometric functions for basis sets and choose a puckering angle as a reaction coordinate. We successfully reproduce VUV/MATI spectrum of thietane (C_3H_6S) with ring-puckering mode. We can assign each peak in the spectrum and calculate Franck-Condon factors and a Boltzmann factor to estimate the intensity of each vibrational transition. As a results, we find that the value of interconversion potential barrier and puckering angle of the thietane cation ($48cm^{-1}$, 18.2°) are much smaller than those of the thietane neutral ($274cm^{-1}$, 26°), where we could suggest that the conformation of the cation should be more planar than the neutral. We apply same calculation method on another ring-shaped molecule, oxetane (C_3H_6O). And we determined the potential barrier of the oxetane cation to almost 0, which means the it should be almost planar.

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A molecular dynamics simulation study on the shear exfoliation of graphene-like nanoplates

장인혁 성봉준*

서강대학교 화학과

The exfoliation of graphene has been one of the most important topics. But it is difficult to produce a few-layered or a monomer graphene of high quality in a large quantity, because there is a strong Van der Waals interaction between stacked graphene layers inside graphite. There have been many conventional methods to exfoliate graphene, but most of them are not sufficiently effective. Contrast to the past conventional methods, shear exfoliation, however, based on the physical exfoliation method, is highlighted because of its high efficiency of producing a few-layered and defect-free graphene in a large quantity without using any harmful and expensive chemicals. We perform molecular dynamics simulations to understand how does the shear force accelerate the graphene exfoliation. We construct the system with two parallel walls, solvent particles and two graphene-like nanoplates stuck to each other. In order to mimic a shear experiment, we apply shear force to the system by pulling upper wall and let the upper wall slide to the x-direction. If the shear force were strong enough to overcome the strong attractive interaction between graphene plates, they would be separated. We analyze the non-equilibrium system by introducing stochastic energetics to find the relation between free energy barrier and perturbation from the shear flow in microscopic scale.

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장소: 일산 KINTEX
발표코드: **PHYS.P-133**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Size-dependent Photophysical Properties of CH3NH3PbBr3 Perovskite Quantum Dots

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연세대학교 화학과

The research area of hybrid organic-inorganic perovskites has grown rapidly due to their superior optical and electrical properties. Although there are some studies of photophysical properties of perovskites, the size dependent photophysical properties of perovskite quantum dots are still scarce.In this study, we have investigated the photophysical properties of CH3NH3PbBr3 perovskite quantum dots with different sizes; 1 (4.2), 2 (7.2), and 3 (9.7 nm). At first we synthesized CH3NH3PbBr3 perovskite quantum dots by controlling the precipitation temperature.[1] After that, we measured Auger recombination time through femtosecond transient absorption experiments and trapping, de-trapping rate, and Auger ionization efficiency through confocal microscope measurements.With an increase in the size of quantum dots, the emission spectra of 1, 2, and 3 are gradually red-shifted; 478, 494, and 515 nm, respectively (Fig. 1). At the same time, the photoluminescence quantum yields increase by 60 to 80 %. Futhermore, the Auger recombination time becomes longer and the Auger ionization efficiency becomes lower with increasing the size of quantum dots (Table 1). These features are attributed to the fact that as the size of quantum dots increases, the density of trap states and the probability of bi-exciton generations is relatively decreased.In conclusion, the photophysical properties of perovskite quantum dots are strongly associated with their sizes. Our studies will provide further insight into the application of perovskite quantum dots by choosing an appropriate size.

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Photoinduced electron transfer dynamics in polydiacetylene with Ru complexes

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Polydiacetylenes (PDAs) are the conjugated polymers which have interesting electronic and optical properties. Upon UV irradiation, self-assembled diacetylene monomers are polymerized to PDAs. Usually, PDAs are blue and have thermochromic or photochromic properties. With these interesting properties, PDAs have been developed for various devices such as light-emitting diodes, photovoltaic cells and chemical sensors. PDAs with a photosensitizer such as Ru complex can be used as effective model systems to study intramolecular electron transfer or energy transfer. Ru complex exhibits strong absorption at 450 nm because of a metal to ligand charge transfer. In addition, an excited singlet state of Ru complex converts rapidly into a triplet state by intersystem crossing and then returns to its ground state by emitting phosphorescence. Phosphorescence lifetime of Ru-PDA is found to be shorter than that of Ru complex resulting from an intramolecular electron transfer from Ru complex to PDA backbone. Here, intramolecular electron transfer dynamics in Ru-PDA were studied by a time correlated single photon counting (TCSPC) method and ultrafast transient absorption (TA) spectroscopy. Spectral features of intramolecular electron transfer dynamics occurring in Ru-PDA were presented and discussed in detail.

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Modeling Studies on the Uptake of Hydrogen Molecules by Graphene (Part II)

김창곤 손창국[1] 박병호 김찬경[*]

인하대학교 화학과 [1]전남대학교 화학교육과

Detailed *ab initio* molecular orbital calculations on the interactions of molecular hydrogen, H_2, with various poly-aromatic hydrocarbons (PAHs) as a model system for graphene were carried out to describe the physisorption phenomenon accurately. The binding energies corrected for the basis set superposition error, E_{bind}(BSSE), were obtained using the optimized geometries at the MP2 level with the SVP and aug-cc-pVDZ basis sets. These results were compared with those obtained at the DFT level of B97D functional, which includes dispersion interaction.

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Removal of CO from hydrogen fuel: A DFT study

Nasir Shahzad 김찬경[1,*]

인하대학교 화학화공공학융합학과 화학전공 [1]인하대학교 화학과

One key challenge for the commercialization of PEMFCs is its strict prerequisite for syngas quality. For hydrogen enrichment and CO removal, water gas shift is widely used. However, this reaction is reversible and cannot remove the CO to the level we are aiming. Double oxidation can achieve this prerequisite. First, oxidize the CO with water gas shift reaction, and then the remaining will be selectively oxidized with air/O_2.We have rationalized the promising catalyst for both these reactions. A single platinum atom containing iron cluster can effectively and selectively perform both water gas shift ($CO + H_2O \rightarrow CO_2 + H_2$) and oxidation reactions ($CO + 1/2O_2 \rightarrow CO_2$) simultaneously in hydrogen rich environment.

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Modeling Studies on the Structure of Carbon Nitride

박병호 오정훈 김찬경*

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Carbon material has become an object of attention. Graphene is a representative material having excellent electrical and physical properties. Many researchers have been working on developing novel carbon materials. Carbon nitride is one of carbon materials made by using nitrogen-containing gases. Within the high-temperature reactor, ordered graphitic carbon nitride can be synthesized, but its structure depends on the source gas. In this study, we considered two types of carbon nitride units as shown in Figure 1. These structures were optimized by using the M11-L functional, which has been known as a good choice for crystal structure optimization due to dual range exchange functional. From the optimized unit structures, several dimer structures were constructed and examined. The fully optimized dimers were compared with the experimental XRD data. The distance between two layers is a primary target. All the calculations were performed by using the materials studio DMol^3 code.

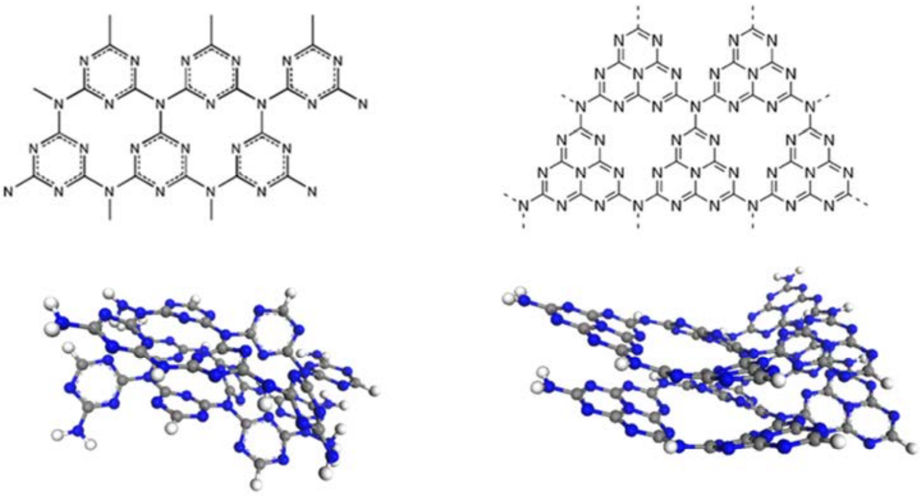

Figure 1. Two types of carbon nitride units (left: trizine-based unit, right: tri-*s*-trazine-based unit) and their dimers examined in this work.

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DFT Study on Competitive Host-guest Interaction

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With the progressive understanding of liquid crystal materials that rely on the interface interactions, optical properties of liquid crystal are attracting attention as a detector for chemicals and biomolecules. In this work, a recently reported liquid crystal sensing system based on the competitive inclusion effect of β-cyclodextrin (β-CD) was studied. Quantum mechanical calculations were applied to study different β-CD inclusion complexes of methyl blue (MB), 4-cyano-40-pentyl biphenyl (5CB), sodium dodecyl sulfonate (SDS), dopamine (DA) and their inclusion processes. The work shows that DA cannot be an analyte for the liquid crystal sensor as it could not compete for the cavity of β-CD with SDS. However, MB molecule can push SDS out of the β-CD cavity so as to induce the change in optical appearance when MB forms a 1:2 inclusion complex.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-139**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Mechanistic Study of Nucleophilic Fluorination Promoted by Tri-*tert*-Butanolamine

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Quantum chemical study is carried out to elucidate the mechanism of S_N2 fluorination using CsF promoted by tri-*tert*-butanolamines. Focus is on the role of the hydroxyl (-OH) and the amine functional groups for accelerating the reaction. Our systematic analysis indicates that the -OH groups form strong hydrogen bonds with F^- to “free” it from the influence of the counter-cation Cs^+. The origin of the experimentally observed noticeable improvement of the promotor efficiency in t-butanol solvent over that in CH_3CN is examined. We show that the coordination of solvent t-butanol molecules as Lewis base on the counter-cation Cs^+. lowers the Gibbs free energy of activation.

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Initial condition issue in the turnover time statistics of enzyme molecules at Mesoscopic Concentrations

정인춘 송상근 김지현 성재영*

중앙대학교 화학과

We investigate how the enzymatic turnover time distribution of systems depends on the number of enzymes and the microscopic reaction dynamics of enzyme-substrate complex. Recently, enzyme kinetics at mesoscopic concentrations to conclude that the mean catalytic rate of a system of enzymes at physiologically relevant mesoscopic concentrations has come to light that does not satisfy the Michaelis-Menten (MM) equation, even though the individual enzyme reaction obeys the MM mechanism. However, that case can only occur the first enzymatic turnover event in N enzyme system under which all the enzymes in the system synchronously start enzyme catalysis at time 0, which means an unrealistic initial condition. We change the initial condition and define the mean enzymatic turnover time satisfies MM equation at any concentration of enzymes in the steady-state as long as each enzyme catalytic reaction occurs in MM mechanism. We confirm correctness of our theory against stochastic simulation results and comparison between the theory and experiment.

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Folding-unfolding thermodynamics of a model globular beta protein

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숙명여자대학교 화학과

Elucidating the factors responsible for protein folding is incompletely understood, therefore of immense scientific interest. With recent advances in computational methodology, especially molecular dynamics (MD) simulations, the mechanism of protein folding and its underlying thermodynamics have become more understandable. However, accurately determining the folding free energy of proteins with unbiased MD simulation protocols remains to be computationally expensive at normal physiological conditions. Interestingly, the free energy of folding of a model helical protein has been recently determined from folded and unfolded state ensembles separately obtained from normal MD simulations.[1] It was obtained by calculating the mean and width of the distributions of protein effective energy (solvent averaged protein-potential energy) of the folded and unfolded states. Further, residual decomposition of the same have indicated the electrostatic interactions, rather than the hydrophobic effect, to be responsible for governing the corresponding folding phenomenon. Hereby, we have investigated with similar protocols, the folding free energy of a model globular beta protein (WW-domain). The corresponding folding free energy is in reasonable agreement with experimental findings. Residual decomposition of the same will further determine each-residue contribution to the overall free energy, hence the dominant interaction responsible for the respective protein folding process.

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Conformationally Resolved Structures of Jet-cooled 2-hydroxyformanilide: IR-depletion Spectroscopy and Computational Studies

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경상대학교 화학과 [1]충북대학교 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 separated that three species coexist in the supersonic jet. Two species among the three are 2-HFA-AC (Anti, Cis) and the other was the 2-HFA-AT (Anti, Trans). The two similar spectra are due to an anharmonic coupling between the peptide group and some ring deformations in the excited state. We speculated that the observance of the IR upstream might come from the contribution of 2-HFA-ST (Syn, Trans). The structures of these conformers are determined by the IR-dip spectroscopy and Franck−Condon simulation. Also, the observed spectra are compared with the predictions of ab initio and density functional theory calculations.

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장소: 일산 KINTEX
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발표분야: 물리화학
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Theoretical study of ethene hydrogenation reaction pathway to ethane using paddlewheel tetrakisacetatodirhodium complex as a catalyst

장효원

순천대학교 화학과

We investigate the reaction pathways starting from several ethene and hydrogen binded binuclear complexes to ethane binded ones by DFT calculation method. The elementary-step energy barriers vary from relatively lower ones involving hydrogen migration from metal to higher ones involving migration of hydrogen from carboxylic group. The present model is distinguished itself from the fact that it can adopt fac-κ^3 conformation for two migrating H's and ethene ligands, which is in contrast to the usual meridional conformation observed when Wilkinson's catalyst is adopted.

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Impact of Copper and Zinc Binding on structure and dynamics of Aβ42 monomer

Subramanian Boopathi 함시현*

숙명여자대학교 화학과

Aggregation of the Amyloid β (Aβ) peptide is an important hallmark of Alzheimer's disease (AD). Zn, Cu and Fe metal ions are found in the amyloid plaques at high concentration, where copper and zinc metal ions directly interact with Aβ peptide but Fe ions were not likely to interact directly with Aβ peptide in vivo. Despite, numerous number of investigation have been put their effort to understand the impact of transition metal ions on the secondary structure changes of Aβ peptide aggregation. Even though, the aggregation mechanism is still elusive. To our best of knowledge, the details of hydrophobic properties of monomer of Aβ42 in the presence of Cu2+ and Zn2+ are still elusive, which correlated with the aggregation behavior. we have to first time investigate the decomposition of the atomic solvation free energy of monomer of Aβ42 in the presence of Cu2+ and Zn2+ in explicit water by combining MD and Decomposition solvation free energy method. Higher solvation free energy has been found in Aβ42–Cu2+ complex, since Cu2+ interactions can enhance the hydrophobicity of Aβ42 peptide in explicit water. Surprisingly noted, the negatively charged residues of Aβ42 peptide play a crucial role to increases the total solvation free energy of Aβ42–Cu2+ complex. This study may shed new light to understanding the impact of Cu2+ and Zn2+ metal ions on the aggregation mechanism of Aβ peptides.

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발표분야: 물리화학
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The investigation of solvolysis mechanism of 2,6-Difluoro-4-methoxybenzoyl chloride

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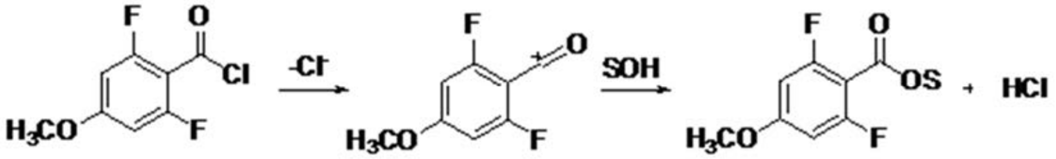
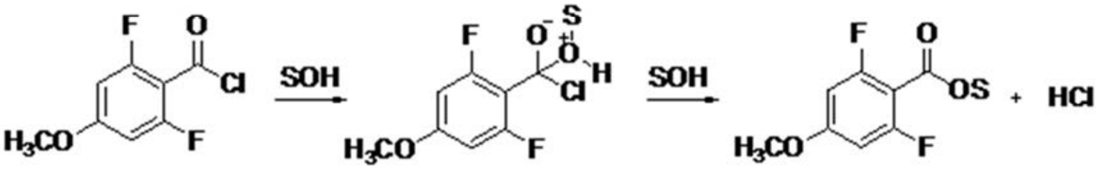
한양대학교 응용화학과 [1]한양대학교 과학기술대학 응용화학과 [2]한양대학교

The measurement of rate constants of 2,6-Difluoro-4-methoxybenzoyl chloride (1) has performed at 25.0℃. The solvents was consisted of the pure ethanol, methanol, 2,2,2,-trifluoroethanol(TFE) and the binary aqueous solutions of ethanol, methanol, TFE. Another binary solvents of ethanol and TFE was used. The rate constants were analyzed by the extended Grunwald-Winstein equation. Also, the activation parameters can support to understand how the reaction go through. From the previous studies of 2,6-difluorobeozoyl chloride (2) has dual SN2 mechanism(associative SN2 and dissociative SN2) and 4-methoxybenzoyl chloride (3) has ionization pathway, it could be expected that the reaction of 1 is the unimolecular pathway. Because the fluoros at orth positions have many electrons and this make the carbon at reaction center more abundant in electricity. Also, the methoxy group at para position push the electrons toward the center carbon. This will makes the unimolecular character be stronger. But, the result is different from the expectation. The plot of data analyzed by simple G-W equation including all solvents has correlation coefficient, R=0.864. And the sensitivity for the solvent ionizing power(m) was 0.35. When applied the extended G-W equation, the R value and the m value are increased as 0.893 and 0.45 respectively and the sensitivity for the nucleohpilicity of solvent(l) was 0.20. Because the rates at the electrophilic solvents(TFE and HFIP aqueous solvents) were extremely fast, the additional work was done. In the nucleophilic system, the solvents with the ethanol, methanol and acetone, the l and m value were 0.79 and 0.50 respectively and R was 0.915 (l/m=1.58). And in the electrophilic system, the binary solution of TFE and water and of TFE and ethanol, the l value was 0.15 and m value was 0.54 with 0.942 as R value (l/m=0.28). Additionally, we gain the activation parameters, the enthalpy is 12.1~14.7 and entropy is -21.5~-9.4. Consequently, the solvolysis of 1 has the dual mechanism. In detail, associative SN2 mechanism in both nucleophilic systems, but the electrophilic system has SN2 pathway, more closer to SN1 mechanism. Also, we compared the result with the data of 2 and 3. When compared the 1 with 2, 1 has para-methoxy substituent at benzene ring. The methoxy group donate the electron to the benzene ring and this makes the carbon of reaction center more stable. Also, compared with 3, the fluorine at ortho- positions, interrupt the detaching of chlorine from the reaction carbon. To sum up, the effects of ortho and para substituents makes the mechanism in 2 ways.



Schem1. Unimolecular pathway



Schem2. Bimolecular pathway

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Investigate the Aggregation Propensity of Tau43 Protein in Water by Molecular Dynamics Simulation and Solvation Thermodynamics Analysis

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숙명여자대학교 화학과

The abnormal aggregation of tau protein into paired helical filaments (PHFs) is considered to be the primary cause of tauopathies. Here, we have performed the fully atomistic, explicit-water molecular dynamics simulations followed by solvation thermodynamic analyses on the minimal sequence of human tau protein, a 43-residue tau fragment (termed Tau43 or PHF43), to identify its structural and thermodynamic characteristics. Tau43 monomer displays fairly localized α-helical and β-sheet structure with the large solvation free energy of the peptide. Remarkably, Tau43 conformational ensembles exhibit structural heterogeneity but thermodynamic homogeneity. Based on the site-directed thermodynamic analysis, we further elucidate the significant contribution of Lysine as well as the hydrophobic residues into regulating the total solvation free energy. Our study thus addresses why Tau43 protein exhibits aggregation-prone characters in aqueous environments.

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발표분야: 물리화학
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Vibronic Spectroscopy of Jet-cooled Indole-3-acetic Acid in the Gas Phase and DFT Calculations

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경상대학교 화학과 [1]충북대학교 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) and UV-UV hole-burning (UV-UV HB) technique in the free jet conditions. As a result, we identified three different conformers of IAA. A combination of infrared-dip, R2PI, UV-UV HB spectroscopy is used to characterize. Further investigation with ab initio and density functional theory calculations of IAA is carried out for the study of potential energy landscapes of IAA.

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발표분야: 물리화학
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Pulsed laser ablation synthesis of alloy nanoparticles in liquids

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경상대학교 화학과

Among various particle fabrication methods, pulsed laser ablation in liquid (PLAL) is currently attracting great interest due to its simplicity and versatility. In this study, a pulsed Nd:YAG laser is used to produce the nanoparticles in solvents. The morphological and optical properties of alloy nanoparticles were characterized by X-ray diffraction, field emission - scanning electronic microscope, energy dispersive spectrometer and high resolution - transmission electron microscope. Synthesized alloy nanoparticles were applied to dechlorinate chlorinated organic compounds under various conditions.

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발표코드: **PHYS.P-149**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Conversion of Methane and Carbon Dioxide to Acetic Acid on Metal-exchanged Zeolite Models: A Theoretical Study

민주은 김용호*

경희대학교 응용화학과

Many Researches have been conducted over the past several years to find a reaction that synthesize useful raw materials using environmental pollutants such as hydrocarbon and oxocarbon/carbon oxide. Recently, the reaction of CH_4 and CO_2 with various catalysts to synthesize acetic acid has been reported, and reaction mechanism for acetic acid synthesis from methane and carbon dioxide using Zn-ZSM-5 zeolite by DFT method was presented. In this study, based on the mechanism, we investigated metal-dependent the catalytic activity of metal-exchanged ZSM-5. The energy and geometry for the synthesis of acetic acid were optimized using the B3LYP.

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장소: 일산 KINTEX
발표코드: **PHYS.P-150**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Transcriptional bursting dynamics from the spectral analysis of intracellular chemical noise

양길석 송상근 김지현[*] 성재영[*]

중앙대학교 화학과

In living cells, the power spectrum of creation rate fluctuation contains rich information about the reaction mechanism and dynamics of the product creation process. However, it is very difficult to directly measure the power spectrum of creation rate fluctuation. Here, we present the general formulation of the power spectrum of product number fluctuation, which can be used to extract the power spectrum of the product creation rate fluctuation. As long as the decay of the product obeys the first-order kinetics, the result is exact regardless of stochastic property of the product creation rate fluctuation, so it is particularly useful in investigating the chemical dynamics of vibrant reaction processes and its consequence in living cells. Application of our result is made to analyze time traces of protein copy number from a stochastic gene expression model of mouse embryonic stem cell. It is shown that the information about the distribution of silent transcription intervals, which is difficult to be obtained by using contemporary experimental techniques, can be extracted from the power spectrum of the protein level fluctuation.

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장소: 일산 KINTEX
발표코드: **PHYS.P-151**
발표분야: 물리화학
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A Comparative Study on the Binding Properties between p53/HDM2 and p53-mimicking Peptide/HDM2

임해리 여진희 함시현*

숙명여자대학교 화학과

Tumor suppressor protein p53 cannot activation of its function upon binding with HDM2. Inhibition of the p53/HDM2 interaction is significant for suppressing the growth of tumor cell. 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 HDM2. Here, we report the structural and thermodynamic characteristics for the binding complex of the stapled p53/HDM2 and cHLH/HDM2. 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 properties between the p53/HDM2, stapled p53/HDM2, and cHLH/HDM2, in order to find the more suitable inhibitor of the p53/HDM2 complex.

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장소: 일산 KINTEX
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발표분야: 물리화학
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Theoretical Studies for the Hydrogen-Transfer Mechanism in the C-H Bond Activation by Non-Heme Iron(IV)-Oxo ($Fe^{IV}O$) Complexes

박수민 Binh Khanh Mai[1] 김용호[*]

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The high-spin iron–oxo species in non-heme enzymes play an important role on many reactions in organism, such as hydroxylation, epoxidation. The C-H activation mechanism by the core parts of these enzymes has long been studied. The biological systems can easily break strong C–H bond with good selectivity. Biomimetic systems of Fe^{IV}–O species have been synthesized by many groups, however, the reactivity of the synthesized complexes are still below expectation. We investigated the comparison between biological (active site model of TauD) and biomimetic (N4Py, Bn-TPEN, TMC-AN, TQA-AN and TMG3tren ligands) systems with employing density functional theory (DFT) calculations to the C–H activation of ethane.

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장소: 일산 KINTEX
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발표분야: 물리화학
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Multiplexed 3D Tracking of Single Upconversion Particles (UCNPs) in Living Cells

고영창 송요한 한영은 이강택[1,*]

GIST 화학과 [1]GIST 물리화학부 화학과

Lanthanide-doped upconversion nanoparticles (UCNPs) are regarded as useful probes for three-dimensional (3D) single-particle tracking in live cells because of a number of advantages: photostability (no photoblinking and no photobleaching), minimized cellular autofluorescence and low level of photo-damage to cells owing to the near-infrared excitation. Recently, we took full advantage of UCNPs to perform 3D real-time imaging thereof (Jo et al, Nanoscale 2015). In this technique, each section image was acquired by wide-field epifluorescence microscopy, and then piled ~15 section images to construct a 3D image, which illustrates the distribution of single UCNPs in the cell. It took ~1 sec to obtain one 3D image and a set of such images were combined and analyzed as a function of time to produce a movie. The drawbacks of our approach were: (1) the software allowed tracking only one trajectory though there are tens of trajectories, and (2) the z-position of the particles determined by Gaussian fitting exhibited artifacts due to the backlash of the step motor used for scanning the objective position. Here, we will report advances in the hardware and software that are used for the live-cell imaging and data analysis. In so doing, we were able to (1) obtain the section images with accurate z positions by introducing electric-piezo mount, and (2) analyze multiplexed trajectories for ~10 particles transported simultaneously in HeLa cells. We will also discuss the mathematical model used for the z-determination of particles.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-154**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

DFT Calculations for Multiple Proton Transfer through Hydrogen Bonded Wire in $ClONO_2$ + H_2O Reactions on the Stratospheric Ice Surface

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경희대학교 응용화학 [1]경희대학교 응용화학과

Multiple proton transfer on the stratospheric ice surface is known to play a key role on the ozone depletion in the Antarctic stratosphere. We calculated rate constants using the variational transition state theory based on the DFT potential energy surfaces. The formation energy of $ClONO_2\cdot(H_2O)_2$ complex and the barrier height for double proton transfer calculated at the MP2/CBS+ΔCCSD(T) level were used as benchmarks to choose the density functional for the rate calculations. This study shows that as the water molecule increases, the energy barrier is lowered and the mechanism changes from the concerted reaction to the multistep reaction with intermediate.

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장소: 일산 KINTEX

발표코드: **PHYS.P-155**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Construction of a new QIT-TOF mass spectrometer

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In order to study structure and function of biomolecules, we are constructing a new ESI (electrospray ionization) – cryogenic QIT (quadrupole ion trap) – TOF (time of flight) mass spectrometer (MS) coupled with laser spectroscopy. Last year we have already constructed QIT and TOF MS. Dipolar ejection capability for conformer-specific spectroscopy has been added and characterized. We have introduced ion source chamber and buffer chamber. The ion source chamber is a 6" CF tube with three 2.75" CF ports for pumping and electrical connections. The ion source is equipped with a stainless steel capillary and skimmer. The stainless steel capillary (ID = 120 µm, OD = 1/8 inch) is a path to transmit and dry charged droplets from atmosphere to vacuum. Skimmer at the end of the capillary is a path to transmit ions to the buffer chamber. The buffer chamber is an 8” CF six way which includes electrostatic 6 lenses. Ions are focused by electrostatic lenses and transmit to QIT chamber. The Buffer chamber is connected with QIT chamber by thin gate valve. We obtained ion signal using TryH+ made from ESI.

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Stable and Size-controlled Perovskite Quantum Dots/Polymer Composite Film

차원희 김동호[1,*]

연세대학교 화학 [1]연세대학교 화학과

Organometallic halide perovskite quantum dots (OHP-QDs) have attracted great attention, showing very high photoluminescence quantum yields (PLQYs) up to 90% and easily controllable narrow-band colors. The emitting color of OHP-QDs can be handled by changing the halide compositions (Cl, Br, I, and/or mixture) and the size of OHP-QDs. However, precise control of the size of the OHP-QDs are very hard and are unstable in ambient environment, which limit their applications in many fields (e.g. laser, display, etc.). Herein, we introduce a new method to synthesis stable and precisely size-controlled OHP (methylammonium lead trihalide, $MAPbX_3$, X = Cl, Br, and I) QDs/polymer film by using polydimethylsiloxane (PDMS) as a template. Using this method, we can not only enhance the stabilities by preventing the direct contact with ambient environment, but also precisely control the size of QDs without using any capping ligands. $MAPbX_3$ QDs/PDMS film synthesized in this work is flexible and transparent which possesses photophysical property of $MAPbX_3$ QDs for more than three months. Also, it showed very narrow peaks of photoluminescence (fwhm ≈ 20 nm) owing to their uniform size, which can be shifted by changing the QD sizes. We think our OHP-QDs/PDMS film enhances the stability compared to conventional OHP-QDs in solution-phase and the emitting color can be accurately controlled which allows its applications in lighting systems, such as light emitting diodes (LEDs).

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Photo-Generating Hydrogen in Water Using Mixed Phase Ultrathin WS_2-CdS Nanocomposite Photocatalyst Under Solar Light Irradiation

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부산대학교 화학과

Transition-metal dichalcogenides (TMD) have emerged as a fascinating new class of noble-metal-free materials for photocatalytic hydrogen evolution from water. Recently, numerous approaches have been established to develop single or few layered TMDs to improve their physical properties. WS_2 has higher intrinsic electrical conductivity than MoS_2, despite having analogous structures. Most efforts are devoted to MoS_2 than WS_2 for photocatalytic applications. Here, we synthesized in-situ and highly efficient few-layered WS_2 nanosheets and exfoliated them to bilayers (i.e., ultrathin) on CdS nanorods (UWC) by a simple ultra-sonication process. The optimized UWC-6 photocatalyst exhibits a tremendous rate of H_2 production of ~185.79 mmol h-1 g-1 using simulated solar light irradiation, with a quantum efficiency of 40.5%. The performance of this photocatalyst is 33 times greater than pristine CdS and 3.5-fold greater than few-layered WS_2-CdS nanocomposite (BWC) photocatalysts. The ultrathin WS_2 nanosheets are long length and discontinuously stacked along the CdS nanorods with high coverage of mixed phase layers. This combination leads to the efficient photo-generation of charge carriers and enhance the surface shuttling properties of the photocatalyst for effective greater H_2 production via active edge sites and superior intrinsic electrical conductivity. The H_2 evolution rate reported herein is much higher than bulk or few-layered WS_2-assisted CdS photocatalysts. To the best of our knowledge, this is the highest H_2 production rate achieved by a WS_2-based CdS photocatalyst for splitting water using simulated solar light irradiation.

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Outstanding photocatalytic hydrogen production over CdS nanorods using noble metal-free copper molybdenum sulfide (Cu_2MoS_4) nanosheets as co-catalysts

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부산대학교 화학과

Charge carrier recombination and durability issues are major problems in photocatalytic hydrogen (H_2) evolution processes. Thus, there is a very important necessitate to extend an efficient photocatalyst to control charge-carrier dynamics in the photocatalytic system. We have developed copper molybdenum sulfide (Cu_2MoS_4) nanosheets as co-catalysts with CdS nanorods for controlling charge carriers without recombination for use in photocatalytic H_2 evolution under simulated solar light irradiation. Effective control and utilization of charge carriers are possible by loading Cu_2MoS_4 nanosheets onto the CdS nanorods. The loading compensates for the restrictions of CdS, and stimulated synergistic effects, such as efficient photoexcited charge separation, lead to an improvement in photostability because of the layered structure of the Cu_2MoS_4 nanosheets. These layered Cu_2MoS_4 nanosheets have emerged as novel and active replacements for precious noble metal co-catalysts in photocatalytic H_2 production by water splitting. We have obtained superior H_2 production rates by using Cu_2MoS_4 loaded CdS nanorods. The physicochemical properties of the composites are analyzed by diverse characterization techniques

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Ultrathin B-doped MoS_2 nanosheets as efficient cocatalyst to improve photocatalytic activity of CdS nanorods for hydrogen production

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Transition-metal dichalcogenides (TMD) are emerged as a promising nonprecious noble metal free catalyst for photocatalytic applications. In TMDs, MoS_2 has been studied widely as a co-catalyst due to enormous performance towards photocatalytic hydrogen evolution. However these catalytic activities of MoS_2 is triggered not maximum S atoms on the basal plane but S atoms on its exposed edges. Immense research was contributed to improve the active S atoms on its exposed edges by conversion of few layers of MoS_2 from many layers and conversion of 1T phase from 2H. The problem here these 1T phases were unstable. So, here we concentrated to improve the catalytically active sites of basal plan existed S atoms. The doping of nonmetal into MoS_2 offers a strategy for the activation of basal plan surface as alternative approach of increasing the density of catalytically active sites. Herein, we report earth abundant few layered boron doped MoS_2 nanosheets decorated CdS nanorods (FBM/CdS) by simple methods for photocatalytic hydrogen evolution under solar light irradiation with lactic acid as hole-scavenger at optimal conditions. The FBM/CdS material exhibits high rate of hydrogen production (196 mmol h^{-1} g^{-1}), the existence of few layered B-MoS_2 nanosheets on the surface of CdS nanorods improves hydrogen production due to their extraordinary active edge sites with superior electrical conductivity. Moreover, the observed hydrogen evolution rate is much higher than that for individual noble metal (Pt), MoS_2-assisted CdS photocatalysts. Considering its low cost and high efficiency, this system has great potential for the development of efficient photocatalysts used in various fields.

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장소: 일산 KINTEX
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Analytic Theory of Non-Gaussian Transport in Disordered Media: Beyond Continuous Time Random Walk

송상근 김지현* 성재영*

중앙대학교 화학과

We introduce analytic theory of Non-Gaussian transport in disordered media based on nonrenewal continuous time random walk (CTRW) model describing stochastic transport in dynamically disordered media. In the model, based on the general relationship between jump event counting statistics and CTRW, we used hidden transition state configuration model with environmental coupling is effected on polymer chain. The mean square displacement of our model could explain the anomalous transport phenomena frequently observed in disordered media, which is proportional to the time squared at short times, the power-law at intermediate times, and linear dependence at long times. Furthermore, the non-Gaussian parameter(NGP) of our model could explain the universal behavior, with 0 value at short and long time, making a unimodal distribution at intermediate time regime. When the time scale of the rate fluctuation in the internal processes is far shorter than the mean jump time, our model reduces to the CTRW with non-monotonic waiting time distribution of which shape depends on . We also discover that the peak time of NGP is similar with the peak time of correlation function of rate fluctuation.

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Homogeneous silver colloidal substrates optimal for metal-enhanced fluorescence

이대두 이재범 송정현 방윤수*

GIST 물리화학부

Fluorescence of dye molecules in close proximity to metal nanoparticles is strongly enhanced by locally induced electric field or energy transfer between fluorophores and nanoparticles. This enhancement effect called metal-enhanced fluorescence (MEF) shows strong dependence on size, shape, composition, and environment of metal nanoparticles. Although numerous results on MEF have been reported, detailed mechanisms of MEF are still controversial.In this work, homogeneous silver colloidal substrates with much narrower extinction profiles than silver island films were prepared in a wide range of particle diameter (70-210 nm) and tested for optimal fluorescence enhancement. Using several dye molecules of distinct absorption and emission properties, the dependence of fluorescence enhancements on the extinction profiles of silver colloidal substrates with distinct size of nanoparticles will be investigated. The emission kinetics measurements by time-correlated single-photon counting and femtosecond transient absorption spectroscopy will also be applied to understand detailed mechanisms of MEF depending on the size of silver nanoparticles.

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발표분야: 물리화학
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Rotational constants and dipole moments of *cis* and *trans* isomers of 2,6-dimethylcyclohexanone from microwave spectroscopy and *ab initio* calculations

장희수 오정진*

숙명여자대학교 화학과

In the range of 6 to 12 GHz, microwave spectrum of 2,6-dimethylcyclohexanone, which has two stereoisomers (*cis-trans*), has been measured by Fourier Transform Microwave Spectrometer. Both b-type and c-type rotational transitions for *cis* isomer, and a-type, b-type, and c-type transitions for *trans* isomer have been assigned to determine rotational constants and centrifugal distortion constants, respectively. The rotational constants of two isomers are consistent with *ab initio* calculation results using Gaussian09. Stark shifts of several transitions have been measured to derive dipole moment components of both *cis*- and *trans*-2,6-dimethylcyclohexanone. Dipole moments of two isomers are also in good agreement with those of equilibrium structures optimized by MP2 calculations.

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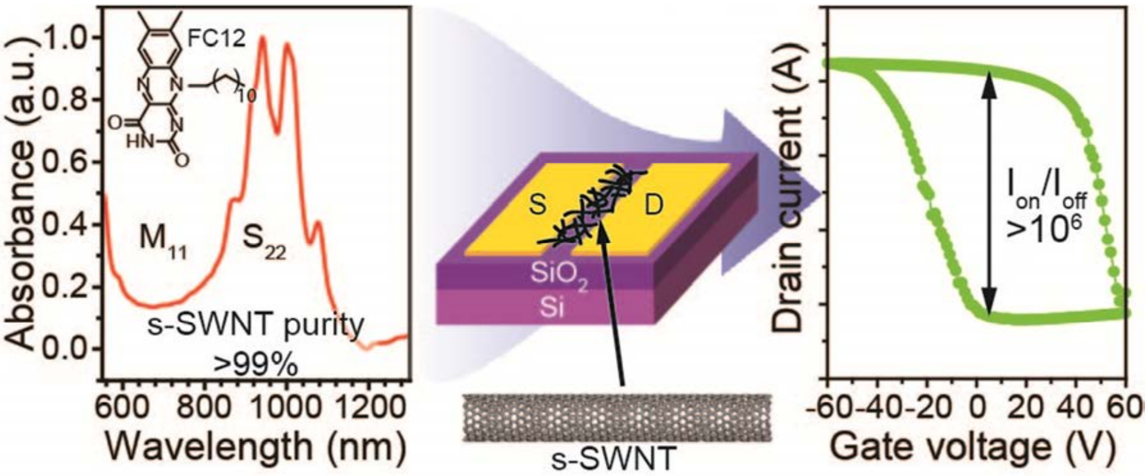
One-step Enrichment Method of Highly Pure Semiconducting Single-walled Carbon Nanotubes by *N*-dodecyl isoalloxazine and Application for Thin-film Transistors

박민석 주상용*

연세대학교 화학과

Semiconducting (s-) single-walled carbon nanotubes (SWNTs) have excellent electrical, optical, and mechanical properties, which can apply them for various optoelectronic applications such as Thin-Film Transistors (TFTs), photovoltaic, chemosensors, electronic skins, etc. Despite their valuable and various applicability, most synthesized SWNTs were mixed with s- and metallic (m-) SWNTs, and they have critical limitation to applicate instantly. Although many researchers try to develop techniques to grow single SWNT chirality recently, the growth throughputs of the methods are still low. For this reason, many researchers developed various method to separate and enrich s- and m-SWNTs from synthesized SWNTs.In this study, we demonstrate a new, and one-step method for separating respective large-diameter s- and m-SWNTs. SWNT dispersion was conducted with *N*-dodecyl isoalloxazine (FC12) as a surfactant. Facile enrichment of s- and m-SWNTs was attained by collecting supernatant and precipitate after sonication and benchtop centrifugation. Especially, a FC12-SWNT dispersion in *p*-xylene condition can be enriched selectively to give s-SWNT with over 98% purity in the supernatant and m-SWNT with 78% purity in the precipitate, respectively. Furthermore, increase the centrifugal force can improve the selectivity of FC12 and elevate larger diameter s-SWNT purity over 99.6% with less carbonaceous impurities, providing purity controllability. These selectivity of FC12 toward s-SWNT originates mainly from photoinduced energy transfer from the isoalloxazine group of FC12 to SWNT. Also, photoreduction properties of FC12 can be used to precipitate and collect enriched SWNT easily. Upon UV irradiation, the isoalloxazine group in FC12 has conformational change to generate bent form, which causes desorption on SWNT surface and precipitate SWNT. A TFT prepared from a dispersion of enriched s-SWNTs was observed to display p-type conductance with average on/off ratio over 10^6 and average mobility over 10 $cm^2/V{\cdot}s$.



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Interface-Confined Anisotropic Thermal Oxidation of 2-Dimensional MoS_2

류예진 류순민*

POSTECH 화학과

Atomically thin planar crystals may reveal novel knowledge on chemical reactions occurring in a low-dimensional space. Despite the importance of surface chemical reactions, interfacial mass transport between 2-dimensional (2D) materials and supporting substrates is not well understood. In this work, we studied substrate-mediated thermal oxidation of 2D MoS_2 supported on SiO_2/Si wafers. Single and few-layer MoS_2 samples were prepared by mechanically exfoliating bulk MoS_2 crystals onto SiO_2/Si substrates. Oxidation reactions were carried out in a quartz tube furnace for a range of temperatures and partial pressures of oxygen. To characterize the changes in morphology, vibrational and electronic structures, Raman and photoluminescence spectroscopies were employed with atomic force microscopy. We observed anisotropic thermal oxidation reactions which formed triangular oxides (TOs) in the bottommost layer and several times smaller triangular etch pits (TEs) in the topmost layer. The former indicates that oxygen molecules diffuse efficiently through the MoS_2-SiO_2 interface at elevated temperatures. Optical second-harmonic generation spectroscopy verified that the TOs and TEs structures are terminated with zigzag edges. MoS_2 crystals on hexagonal boron nitride and thick graphene did not form TOs, which indicates that the oxidation is greatly enhanced in direct contact with the SiO_2 substrates. We will discuss the possible roles of SiO_2 substrates and other various aspects of the oxidation reaction and oxidized MoS_2 crystals.

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장소: 일산 KINTEX
발표코드: **PHYS.P-165**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrochemical Ambient Charge Doping in Single-Layer WS_2 Supported on SiO_2 Substrates

강하늘 류순민*

POSTECH 화학과

Understanding charge transfer (CT) between two-dimensional (2D) crystals and molecules is crucial for the fundamental research and future applications of 2D material systems. Despite recent surge on this research subject, however, the roles of the interface formed by supporting substrates and their surfaces have not been investigated. In particular, ambient water may form a medium on hydrophilic surfaces for electrochemical reactions with oxygen in the air. In this work, we investigated the CT interaction of single-layer WS_2 with the proposed redox couple of O_2/H_2O serving as a hole dopant. Photoluminescence (PL) and Raman spectra were obtained for mechanically exfoliated WS_2 mounted in an gas-controlled optical cell. The enhancement in exciton PL attributed to O_2-mediated CT was higher on SiO_2 than that on h-BN (hexagonal boron nitride) substrate, which supports the CT model based on the electrochemical redox reaction. Since this result also suggests efficient interfacial diffusion of oxygen, additional experimental methods are being developed for spatially-resolved kinetic studies. We will further discuss detailed photophysics of charged excitons (trions) and possible roles of defects in the observed CT reactions.

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발표분야: 물리화학
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Stimulated Raman spectrum on trans-Stilbene

강동구 박승혁 김상규*

KAIST 화학과

We have constructed an optically prototypical setup that is named femtosecond stimulated Raman spectroscopy (FSRS). This technique is able to collect excited-state vibrational spectra on the femtosecond time scale whose frequency resolution limits are completely separate from the time resolution. We checked the stimulated Raman spectra on trans-stilbene solution by using a fundamental narrow-bandwidth picosecond Raman pump pulse and a white-light continuum femtosecond Raman probe pulse. To investigate ultrafast structural dynamics on condensed-phase, we try to set the experimental condition that are sub 50 fs time resolution and sub 10 cm^{-1} frequency resolution with three optical pulse.

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발표분야: 물리화학
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Catalytic performance of Fe_2O_3 nanoparticles deposited on mesoporous Al_2O_3 bead toward toluene total oxidation

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성균관대학교 화학과 [1]상명대학교 화학에너지공학과

By temperature-regulated chemical vapor deposition (TR-CVD), Fe_2O_3 and NiO were deposited on mesoporous Al_2O_3 bead (size of ~ 1 mm) using $Fe(Cp)_2$, $Ni(Cp)_2$ as metal precursor and oxygen contained in air as oxidizing agent, respectively. In the case of Fe_2O_3/Al_2O_3, Fe_2O_3 nanoparticles were distributed even at the core part of Al_2O_3 bead, while NiO/Al_2O_3 showed narrow distribution of NiO nanoparticles with only shell part which of depth were ~50 μm. After post-annealing of these catalysts under air at 450-750 °C, these catalysts were used for total oxidation of toluene in the reaction temperature range of 150-350 °C. Fe_2O_3/Al_2O_3 showed significantly higher catalytic activity than NiO-based catalysts, which can be attributed to the wide distribution of Fe_2O_3 nanoparticles, i.e., very small catalytically active nanoparticles are distributed in the entire structure of the mesoporous supporting material. 100% conversion of toluene into CO_2 with a long-term stability of the catalytic activity was realized at 350 °C using Fe_2O_3/Al_2O_3 under both dry and humid conditions with a toluene concentration of 10,000 ppm in the feed gas. Our Fe_2O_3/Al_2O_3 catalysts are active for toluene oxidation, and stable upon annealing at high temperature, showing that one can use our Fe_2O_3/Al_2O_3 as a component of catalytic converter of harmful volatile organic compounds.

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장소: 일산 KINTEX
발표코드: **PHYS.P-168**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Investigation of humidity effect on photocatalytic mineralization of acetaldehyde over TiO_2 surface under UV light irradiation

우태균 김영독* 서현욱[1,*] 김일희 한상욱 차병준 김호종 박찬흠 정재환

성균관대학교 화학과 [1]상명대학교 화학에너지공학과

Photo-catalytic mineralization of acetaldehyde on the surface of TiO_2 films under UV light irradiation were studied at various humidity conditions (0, 16.8, and 33.6 relative humidity %) using a high vacuum chamber equipped with online gas-chromatography as a batch-type reactor. Competitive adsorption between acetaldehyde and water molecules on TiO_2 surface under dark condition was observed and higher humidity level reduced both reaction rates of acetaldehyde consumption and CO_2 evolution. The CO_2 evolution rate was much more influenced by increasing humidity level than the acetaldehyde removal rate, particularly over the certain level of humidity. We revealed that it was the oxygen molecules that majorly mediated the total oxidation of acetaldehyde rather than water molecules under our experimental conditions. Our experimental observation can be explained as follows. Photo-catalytic conversion of acetaldehyde to CO_2 was boosted by the presence of free active sites ensemble which were available to approaching oxygen molecules near the adsorbed acetaldehyde under dry condition. The adsorption of oxygen molecules on those free active sites were disturbed by the competitive adsorption of H_2O molecules with O_2 molecules on the active sites of TiO_2 surface under humid conditions. As a consequence, photo-catalytic reaction rate of acetaldehyde mineralization over TiO_2 surface under UV light irradiation decreased.

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Assembly of PDMS/SiO_2-coated PTFE and ACF: For Development of a protective layer to prevent liquid and gaseous contaminants

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성균관대학교 화학과 [1]상명대학교 화학에너지공학과

Polytetrafluoroethylene (PTFE) membrane was dip-coated with a hexane-based solution containing polydimethylsiloxane (PDMS)-coated SiO_2 nanoparticles and fluidic PDMS as a binder. PDMS-coated SiO_2 deposited on PTFE membrane surface provided a superhydrophobic characteristic with a water contact angel exceeding 160^o. We aimed to develop a new protection layer against aqueous and gaseous contaminants by combining PDMS/SiO_2-coated PTFE and activated carbon fiber (ACF); superhydrophobic property of PDMS/SiO_2-coated PTFE repels the aqueous contaminants while gaseous contminants could be removed by adsorption on ACF with high surface area. The adsorption behavior of dimethyl methylphosphonate (DMMP) on our novel assembly structure was investigated by conducting breakthrough experiments using a continuous flow-type system connected to a gas chromatograph (GC) and the humidity effect on DMMP adsorption was studied at two different humid conditions, 16 and 32 RH%, respectively. After the breakthrough experiments, the ACFs were taken out from the reactor and the surfaces were immediately analyzed with Fourier-transform infrared spectroscopy (FT-IR) with a view to provide insights into the DMMP adsorption states and amount of DMMP remaining on the ACF surface. Our result implies that even though DMMP can be removed efficiently by our novel structure under various humidity conditions, adsorption mechanism is dependent of the humidity conditions. Based on these results, we suggest the following scenario; DMMP can irreversibly chemisorb on ACF under dry conditions, whereas under humid conditions, DMMP cooperatively adsorb with water vapor. The DMMP co-adsorbed with water vapor is mostly reversibly adsorbed.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-170**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Computation study on the structural and optical properties of a light-responsive helical nanostructure

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울산대학교 화학과 [1]*Department of Chemistry and Biotechnology, Tottori University*

Light-responsive helical nanostructures have increasingly received much attention due to their fascinating optical properties [1]. In this study, we successfully synthesized a novel type of helical nanostructure which consists of achiral trigonal molecules in a manner of helical assembly. The UV-Vis spectroscopic study presented the hypsochromic shift depending on the polarity of solvent medium. The time-dependent density functional theory (TD-DFT) calculations with self-consistent reaction field approximation revealed that the experimentally observed solvatochromism can be explained by the geometric change near core-benzene moiety. In addition, a symmetry breaking of three-fold helical morphology observed in NMR spectroscopy was suggested as due to the trans-cis conformational change in an azo-moiety by means of DFT calculations.

1.M. Han, S. J. Cho, Y. Norikane, M. Shimizu, and T. Seki, Chem. Eur. J. 22, 3971 (2016).

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장소: 일산 KINTEX
발표코드: **PHYS.P-171**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Polarized Raman Spectra of Layered $CrPS_4$ Crystal and its 2-Dimensional Subsystems

김수진 류순민*

POSTECH 화학과

Chromium thiophosphate ($CrPS_4$), a monoclinic crystal of C_2 space group, is a ternary layered semiconductor with an optical bandgap of 1.4 eV and exhibits antiferromagnetism below 36 K. Despite its potential in optoelectronic and magnetic applications, its lattice vibrations have not been studied. In this work, we performed a polarized Raman spectroscopy study of bulk and few-layer $CrPS_4$. High quality crystals grown by the chemical vapor transport method were mechanically exfoliated into thin crystals with thickness ranging from single-layer to tens of nm. Raman spectra of few-layered crystals exhibited systematic frequency progressions with respect to the bulk as a function of thickness due to quantum confinement effects. Polarized Raman spectra were obtained in parallel and cross configurations, where the polarization of the Raman signal was parallel and perpendicular to that of the excitation beam, respectively. Among 33 Raman active modes (16 A and 17 B) at the Brillouin zone center, 11 (9) peaks observed in the parallel (cross) configuration were assigned as A (B) modes. To determine the polarizability Raman tensor value, the angular dependence of A and B modes are under a systematic investigation by rotating crystals with respect to the excitation polarization. We will further discuss the dependence of the polarized Raman spectra on the excitation wavelength and crystal thickness.

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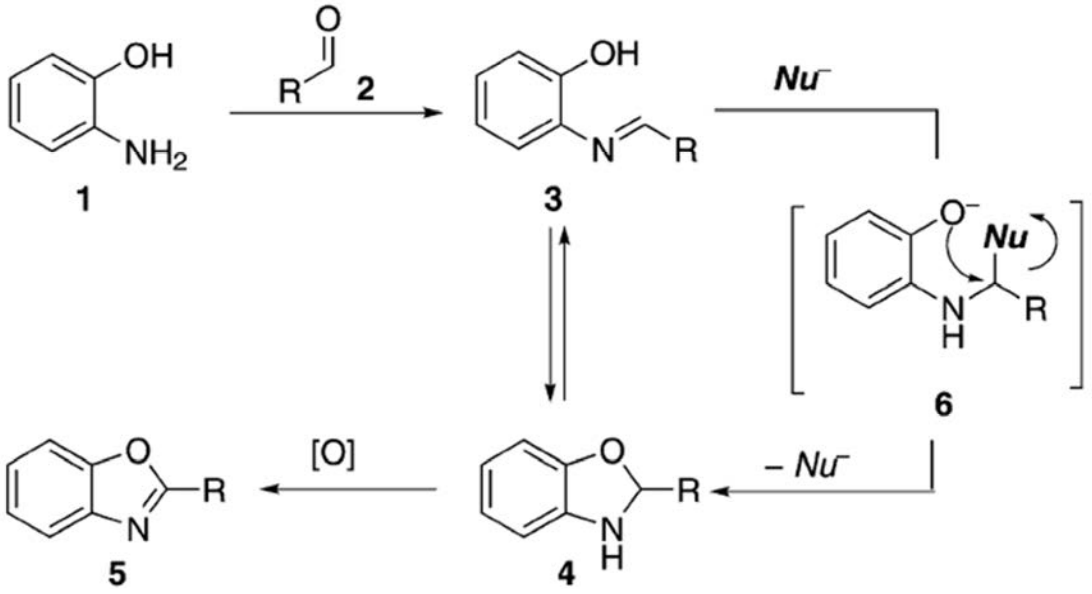
장소: 일산 KINTEX
발표코드: **PHYS.P-172**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Mechanisms of Metal-Free Aerobic Oxidation to Prepare Benzoxazole Catalyzed by Cyanide

정태섭 채영석 임채호 천철홍* 곽경원*

고려대학교 화학과

Benzofused azoles are important building blocks in therapeutically active compounds, natural products, and functional materials. There are 3-step sequences to synthesize the benzoxazole molecules (Scheme 1). First, an aniline is condensed with an aldehyde molecule, intermediate Schiff bases is formed . Next step is an equilibrium step between the Schiff base and benzoxazoline. This step is one of the cyclization reaction. Finally, benzoxazoline is dehydrogenated by oxygen gas, benzoxazole products is formed . Recently, Prof. Cheon’s group proposed a cyanide based powerful metal-free catalyst for synthesis of benzoxazole molecules and they asserted that the cyanide attacks the carbon of imine and enables the orbital interaction between σ* of C-CN and the lone pair on the X-group (Baldwin's 5-exo-tet rule). However, Chen et al. in Nankai University, argued this mechanism computationally. They reported the activation energy of this mechanism is too high for the facile preparation of benzoxazole compounds on room temperature. Therefore, we will show some computational results to verify the mechanisms using Gaussian 09 program. And we will introduce some IR spectrum during the reaction.



Scheme 1. Working hypothesis.

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장소: 일산 KINTEX
발표코드: **PHYS.P-173**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structures and Electronic Properties of Si_nC_n (n = 1 - 6) Clusters using *ab initio* Monte Carlo Simulations and Density Functional Theory Calculations

배균택* 정유경[1]

충북대학교 사범대학 화학교육과 [1]충북대학교 화학교육과

Silicon Carbide(SiC) is the exclusive chemical compound of carbon and silicon. SiC clusters show highly resistant, good mechanical properties, in high temperature. In this study, we obtained the most stable structure in neutral and charged Si_nC_n (n = 1 - 6) clusters using *ab initio* Monte Carlo simulations and density functional theory calculations. We obtained structural and electronic properties including bond lengths and bond angles, atomization energies, electron affinities, ionization energies, HOMO-LUMO gaps, and Mulliken charges.

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장소: 일산 KINTEX
발표코드: **PHYS.P-174**
발표분야: 물리화학
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Structures and Electronic Properties of Cu_nSn_n (n = 1 - 6) Clusters using *ab initio* Monte Carlo Simulations and Density Functional Theory Calculations

배균택* 신주희[1]

충북대학교 사범대학 화학교육과 [1]충북대학교 화학교육학과

The copper and tin (Cu/Sn) interface plays an important role in micro-electronic industries such as catalyst, semiconductor, and corrosion. We calculated structures and electronic properties of CuSn clusters and compared with the experimental data. We found stable neutral and charged Cu_nSn_n clusters (n = 1 - 6) using *ab initio* Monte Carlo Simulations and density functional theory calculations. We examined bond lengths, bond angles, atomization energies, ionization energies, electron affinities, second differences in energies and Mulliken charges for Cu_nSn_n clusters (n = 1 - 6)

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장소: 일산 KINTEX
발표코드: **PHYS.P-175**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Vibrational population relaxation of the methyl formate in CH_3CN solution

김성흔 신주향[1] 박성철[1] 임만호[1,*]

POSTECH 포항가속기연구소 [1]부산대학교 화학과

Ultrafast mid-IR pump-probe spectroscopy was used to study the vibrational relaxation dynamics of a transient C=O stretching vibrational mode of HCO2CH3 in CH3CN solution at room temperature. . Time-resolved spectra after excitation of the C=O stretch mode of HCO2CH3 show a new absorption, which arises from an intermediate state. The amplitude of the intermediate state initially grows and then decays with the pump-probe delay time. The bleach and the transient excited-state signals have nonexponential relaxation behaviors and the kinetics of the bleach is somewhat slower than that of the transient excited-state absorption. From this study, we will propose the kinetics model, which can explain the relaxation pathways of vibrational energy after excitation of the C=O stretch mode of HCO2CH3.

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발표분야: 물리화학
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Complete Basis Set Limit of CCSD(T) Calculation for Potential Energy Curve of the OH Stretching of a Water Molecule

전기영 양민오*

충북대학교 화학과

응축상 물의 구조와 동역학을 이해하는 데 있어, 수소결합에 의해 주변 분자구조에 민감한 OH 수축 진동 분광학 실험이 활발히 진행중이다. 여기서 위 실험결과 얻어진 스펙트럼에 대한 이론적 해석이 필요하며, 이를 위해 분자들의 병진운동과 회전운동은 고전역학적으로, 진동운동은 양자역학적으로 기술하는 mixed QM/CM 이론이 사용된다. 양자역학적으로 나타내어지는 OH 수축 진동운동으로부터 포텐셜 에너지 커브를 얻어내고 슈뢰딩거 방정식을 풀면, 위에서 언급한 스펙트럼을 재현하기 위해 필요한 다양한 바깥 물 분자 구조들과 상호작용하는 한 분자의 OH 진동과 관련된 물리량들이 나온다. 이러한 진동 물리량들을 구하는 과정의 정확성을 담보하기 위해, 원칙적으로는 포텐셜 에너지를 높은 ab initio 방법으로 계산해야하지만 시간상 실행할 수 없으므로, 이를 대체할 수 있는 낮은 수준의 이론이 필요하다. 어떤 이론을 쓸 지 결정하기 위해서는 benchmark 한 값이 필요하다. CCSD(T) 등의 특정 CI 이론들이 수많은 양자계산 결과를 정확히 준다고 널리 알려져 있으나, complete basis set(cbs)을 쓰지 않았을 경우 basis set error 가 추가로 발생한다. 이 basis error 를 최소화하기 위해 1998 년 Truhlar 등이 쓴 논문들이 있지만, 이는 여러 분자에 대한 계산결과를 종합한 것이기 때문에 물 자체의 에너지를 구하는데는 정확성이 다소 떨어질 수 있다. 이번 연구에서는 물에 대한 에너지를 CCSD(T)/cbs 방법으로 정확히 구하기 위한 시도를 한다.

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발표코드: **PHYS.P-177**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Role of Chloride as Dopant on the Bright Trion States in Cesium Lead Iodide (CsPbI3) Perovskite Quantum Dots

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연세대학교 화학과

At the single molecule level, most semiconductor nanomaterials show a binary-like “on-off” transitions in the PL with a significant variability in duration which can last up to several seconds at a time. These PL interruptions, so called blinking, pose a limitation on potential applications as efficient and reliable nanoscale emitters. It has been studied widely in zero-dimensional QDs and scarcely in one-dimensional systems. Charging model have been proposed as the most likely mechanisms responsible for the PL blinking; this hypothesis has been supported by lots of experimental observations most remarkably by the fact that illumination can lead to ionization of single NC. Charge trapping to a surface or lattice-defect state leaves a single unpaired charge in NC core. Photon absorption when the particle is in this state results in a both positive trion (positively charged exciton) and negative trion (negatively charged exciton). The NC is unable to radiate due to efficient nonradiative Auger decay while in one of these charge-separated state. However, currently, it has been observed that some types of nanomaterials display an additional transition state that act as an intermediary (grey) between the “on” and “off” states. In this work, we have observed and identified bright trion state in Cl-doped CsPbI3 PQDs. The observation of bright trion state allows the determination of properties in chloride dopant in CsPbI3 PQDs that are otherwise hidden.

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발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Experimental and simulation study of 3-methylthioanisole: carrier gas dependent methyl group internal rotation

이희성 김상규*

KAIST 화학과

As an extension study of dynamic resonance for thioanisole, methyl group substituted thioanisole could be an issue.We observed carrier gas dependent REMPI (resonance enhanced multiphoton ionization) spectra for 3-methylthioanisole and analyzed results. We used 1D hindered rotor Hamiltonian. By virtue of the Stark deflection profile and hole-burning spectroscopy, we did assignment of the two different conformers.In addition, we assumed that there are two conformers in the ground state 3-methylthioanisole. Energetically lower conformer might collide with the heavy carrier gas more effectively. Because Ar mass is nearly double of Ne mass, Ar backing condition could make 3-methylthioanisole (3MTA) be existing as trans conformer in ground state. This was comparable to the data from *Gaussian*09.To be specific, we made a model to describe the methyl internal rotation. It could be possible that the 1D hindered rotor Hamiltonian describes the methyl internal rotation if there is no significant vibration-torsion coupling. For the 3-methylthioanisole, C_{3v} point group was chosen, and there might be a- type (0a→na) or e- type (1e→me) transitions (n=0,3,6,...; m=1,2,4,5,7,8,...) from ground to excited states. We made two 31x31 Hamiltonian matrices and used three fold (V_3) and six fold (V_6) barriers from quantum calculations. Diagonalization of the aforementioned matrices manifested eigenvalues for the ground and excited states respectively. Franck-Condon factors for the transitions of methyl internal rotation were calculated by multiplying every pair of eigenvector elements followed by sum of them.In conclusion, we observed carrier gas dependent spectra for 3-methylthioanisole and assigned the corresponding methyl internal rotation peaks.

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장소: 일산 KINTEX
발표코드: **PHYS.P-179**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The pump-probe study of Intraband of OLA-HgS Quantum dot

임준형 윤빛나 정광섭 곽경원 조민행*

고려대학교 화학과

The colloidal quantum dots(CQDs) can be utilized in laser source, LEDs, quantum computation and many more. Especially, the intraband transition of CQDs is in the spotlight because it allows reaching mid-IR regime and it can be used for MIR laser sources or photoedetector. Unfortunately, its application is limited by too fast decay of excited states of CQDs which is usually explained by Auger processes. In these days, there are opinions that this fast decaying is from not only the Auger process but also the electron cooling. In our work, we did IR pump-probe measurements of HgS Quantum dots. To study the dynamics of pure conduction band, the electronic doping of HgS CQDs was done by using organic ligand(Oleylamine). Therefore, our observation is confined in intraband transition of conduction band and there will be no trap states. Interestingly, the results show wavelength(or size)-independent, sub-ps dynamics and interesting decaying pattern. We believe this result can be explained by cooling-down of hot electron.

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Early Detection of Pancreatic Cancer on Atomically Flat Single-crystalline Gold Nanoplates

이미연 김봉수*

KAIST 화학과

Pancreatic cancer is one of the most malignant tumor with a dismal prognosis because of lack of any signs or symptoms at an early stage. Glypican-1 is overexpressed in primary pancreatic cancers that offer a potential new biomarker for enabling early diagnosis and screening tool. For the ultrasensitive glypican-1 detection, we present a surface-enhanced Raman scattering (SERS) based detection method using [Au nanoplate + protein G] complex and Au nanoparticles. Here, we combined cysteine tagged protein G which immobilizes anti- glypican-1 with correct orientations to an ultraflat, ultraclean and single-crystalline Au nanoplates through Au-S bonding. Especially, atomically smooth single-crystalline Au nanomaterials is very suitable to fabricate reproducible sensitive sensors. And we confirmed a high surface coverage of anti-glypican-1 supported by protein G on the Au nanoplates from atomic force microscopy measurement. Interestingly, the well-ordered anti-glypican-1 by combination of the Au nanoplate and protein G show the great selectivity toward non-target compounds at their concentration commonly found in blood. Moreover, SERS sensor prepared by assembly of [Au nanoplate + protein G] complex and Au nanoparticles can detect glypican-1 with 10 aM of detection limit. The ultraflat Au nanoplate might be the best substrate to immobilize protein G without negative effects caused by surface roughness. We expect that the detection platform employing the complex of single-crystalline Au nanoplates and protein G can be used in various high-sensitive biosensor applications which employ the IgG typed antibodies.

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발표코드: **PHYS.P-181**
발표분야: 물리화학
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Synthesis of upconversion nanoparticles (UCNPs) for multicolor imaging

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Lanthanide-doped upconversion nanoparticles (UCNPs) have attracted huge interest in the field of bio-imaging because of their unique and fascinating optical properties. In addition, Yb3+-sensitized UCNPs emit photons with various wavelengths upon excitation at 980 nm. The wavelength can be adjusted by varying the composition of the lanthanide ions. Here, we report on the synthesis of core-shell UCNPs for multicolor imaging. We adopted a solvothermal method in order to enhance the mono-dispersity and the quality of nanoparticles. Of the emitter dopant ions, Tb3+-Eu3+ and Tm3+-Er3+ pairs display excellent spectral behavior suitable for multicolor detection. We discuss the possible application of multicolor imaging for identifying cell types and cancer diagnosis.

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장소: 일산 KINTEX
발표코드: **PHYS.P-182**
발표분야: 물리화학
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Enhanced Photoelectrochemical Properties of (040) Crystal Facet Engineered BiVO4 Photoanode

강영수* 지소현

서강대학교 화학과

Artificial photosynthesis is generating solar chemical fuels by using incident solar-to-energy conversion using semiconductor cell which has the cathode and the anode. When external solar energy corresponding 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 compartment. To reduce the carbon dioxide into liquid fuels, protons and electrons have to be supplied at the same time as one pot reaction from anode compartment.Here, (040) crystal facet controlled BiVO4 is used for photoanode. 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 does not have enough energy for water splitting. Although UV light has sufficient energy but it has a portion less than 5% in sunlight. Additionally it is non-toxic and has low photo-corrosion property. But experimental data value can not reach to theoretical one because of its several limiting factors like high recombination probability of photo-generated electron-hole pair and slow charge transfer kinetics for water oxidation. To overcome these limitations, method of crystal facet engineering has been tried. Because the exposed atoms on surface of BiVO4 crystals are altered depending on the morphology of semiconductor, it influences on photocatalytic performance of BiVO4 crystals. 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 originated from increased conductivity of (040) crystal facet engineered BiVO4. This (040) crystal engineered BiVO4 was synthesized by using hydrothermal method.

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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 methanol. 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 with a direct band gap of 2.26 eV shows the high capability of reducing CO2 to highly reduced liquid product. 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 reaction.

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발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Modification of WO3 Nanoparticles for Photochemical CO2 Reduction into Hydrocarbon Fuels

<u>Zheng jin you</u> 강영수*

서강대학교 화학과

WO3 has attracted a lot of interest due to its photosensitivity, good electron transport properties, and stability against photocorrosion.[1-4] Its valence band is positive enough for water oxidation reaction; however, the conduction band minimum of bulk WO3 is about 0.4 V (vs NHE at pH = 0) below the redox potential for water splitting to H2 and CO2 reduction to hydrocarbon fuels such as CH4 and CH3OH; It is difficult for WO3 nanoparticles to reduce water and CO2. Therefore, WO3 should be modified for adjusting its photocatalytic properties. The photocatalytic reactivity of a semiconductor photocatalyst is affected by its surface environment such as surface electron density and atomic structures.[2,4] The surface properties tunable by crystal facet engineering, doping and constructing heterostructure can easily adjust the properties of the semiconductor, such as electronic band structure, surface energy and surface active sites, adsorption of reactant, and selection of products. The WO3 nanoplates with (002) facet exposing, Bi-doped WO3, NaxWO3 and WO3@TiO2 core-shell structure powders were synthesized and used for photochemical CO2 reduction. The hydrocarbon fuels such as CH3OH, HCHO, CH3CHO were produced.

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발표코드: **PHYS.P-185**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced Photocatalytic CO_2 Reduction Ability of $BiVO_4$ with Highly Uniform Octahedral $NiFe_2O_4$ Co-Catalyst

박홍렬 강영수*

서강대학교 화학과

Due to the anthropogenic CO_2 emission, the concentration of atmospheric CO_2 level is sky-rocketing.[1] To alleviate the atmospheric CO_2 level, scientists have focused on artificial photosynthesis which is the reaction that converts CO_2 gas into utilizable fuels. As a part of this research, several disquisitions which treat the ability of photochemical CO_2 reduction with $BiVO_4$ were reported. [2,3] Here, ultra-uniform monodispersed octahedron $NiFe_2O_4$ NPs were loaded as co-catalyst in $BiVO_4$ particles. $NiFe_2O_4$ is p-type semiconductor, thus it could make P-N junction with n-type semiconductor, $BiVO_4$. The conduction band and valence band potentials of $NiFe_2O_4$ are higher than the bands of $BiVO_4$, therefore the $NiFe_2O_4$ composite could achieve an enhanced charge separation ability by electron and hole transfer. Furthermore, the solar light absorbance of $NiFe_2O_4$ is extended from UV to near-IR region. It means that $NiFe_2O_4$ could be a complementary antenna to receive broad range wavelength of solar light for artificial photosynthesis with $BiVO_4$, which could absorb wavelength shorter than 550 nm. And so on, the unique octahedral structure of deposited $NiFe_2O_4$ could show better capability for water splitting. Spinel ferrite octahedron is enclosed with 8 faces, and all of them has (111) facet. According to the previous calculation, activation energy of $NiFe_2O_4$ for water adsorption is quite low.[4] Therefore it could be expected that $NiFe_2O_4$ deposited photocatalyst particles would shows better efficiency in artificial photosynthesis. Octahedron $NiFe_2O_4$ NPs were obtained by modifying monodispersed nanoparticle synthesis method of Gupta.[5] The deposition was achieved by adding obtained $NiFe_2O_4$ NPs into $BiVO_4$ particles synthesis process.[6]

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장소: 일산 KINTEX
발표코드: **PHYS.P-186**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Photocatalytic CO2 Reduction by g-C3N4 nanosheets/CuInS2/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 the methods to induce photocatalytic CO2 reduction to hydrocarbon liquid fuels under solar light irradiation. Due to its high stability and narrow band gap, g-C3N4 is novel, nonmetallic semiconductor. g-C3N4 nanosheets have different properties and photocatalytic activity from bulk g-C3N4 mainly in two aspects. First, the electron and hole mobility in the nanosheets is significantly larger than that in the bulk. Second, the surface area of the nanosheet is larger than the bulk, which is also very important for photocatalyst. In addition, g-C3N4's nitrogen can adsorb the CO2 molecule through the Lewis acid base reaction, so absorbed CO2 molecule can be easily activated to higher energy state. Copper induim disulfide (CIS) is an attractive candidate material as a photocathode material because it has visible light driven photocatalytic property with optimal band gap, the high optical absorption coefficient, relatively low cost and non-toxic property. For making CIS and g-C3N4 nanosheet composite film, the obtained g-C3N4 nanosheet is dispersed in isopropanol. And dispersed g-C3N4 was subjected to centrifugation to remove any unexfoliated g-C3N4. And then flake-like solution was spin-coated on the CIS film at a several rpm. The prepared g-C3N4/CuInS2 will be coated with Nafion to have proton transfer rapidly, so one-pot reaction media, during CO2 reduction reaction.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-187**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Synthesis of SmCo5 Nanoparticles from the Assembly of Nanowire Shaped Co/Sm2O3

MaHaoXuan 강영수*

서강대학교 화학과

Hard rare earth permanent magnetic materials with high ferromagnetic performance have attracted much attention for several applications. SmCo5 based magnets with small size and good magnetic properties have been developed and applied for many scientific fields. In order to improve the properties of SmCo5, we report a facile synthesis of ferromagnetic SmCo5 nanoparticles from Co/Sm2O3 nanowires. Using the self-organized cobalt nanowires with dimensions of 100 - 200 nm, the Sm2O3 layer was deposited on the surface of Co nanowire. With a controlled reduction of Co/Sm2O3 as core/shell structured composite protected by CaO matrix, 100 - 200 nm SmCo5 nanoparticles were obtained. This synthesis route also can be further utilized in the synthesis of other kinds of nano-structured magnet.References[1] H. X. Ma, C. W. Kim, D. S. Kim, J. H. Jeong, I. H. Kim and Y. S. Kang, Nanoscale., 2015, 7 , 8016–8022.[2] K. Gandha, K. Elkins, N. Poudyal, X. Liu and J. P. Liu, Sci. Rep., 2014, 4, 5345.[3] Y. Hou, Z. Xu, S. Peng, C. Rong, J. P. Liu, S. Sun. Adv. Mater., 2007, 19, 3349-3352.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-188**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Stable structure of hydrated protons on Pt surface

김영순 강헌*

서울대학교 화학부

The nature of hydrated protons at an electrolyte/electrode interface is a fundamentally important topic in wide variety of scientific research, including heterogeneous catalyst, corrosion, and electrochemical processes in acidic environment. A key electrochemical step of hydrogen evolution reaction (HER), which is the most studied electrode reaction, is the conversion between proton in solution and atomic hydrogen adsorbed on electrode surface.[1] A question in this reaction is whether hydrated protons exist on a Pt electrode as surface-bound ions or the charge transfer occurs between an electrode and “non-specifically” adsorbed hydrated protons. However, understanding the nature of this process is experimentally difficult to identify hydrated proton structures at the buried interface in electrochemical environment. Here, we explored the stability of hydrated protons on a Pt surface in ultra-high vacuum (UHV) by coadsorption of atomic hydrogen and water layer. Studies based on mass spectrometry and reflection absorption infrared spectroscopy (RAIRS) show clear evidence that hydrogen atoms can be ionized into hydrated protons on a Pt(111) surface.[2] The preferential structures of surface-bound hydrated protons on Pt(111) were identified as multiply hydrated protons ($H_5O_2^+$, $H_7O_3^+$ and $H_9O_4^+$) rather than as hydronium (H_3O^+) ions. This indicates that this structure might be two-dimensional Eigen-like and Zundel-like structures on metal surface. The surface-bound hydrated protons were transformed to a different structure by adding water adlayer, which simulated interfacial water in electrochemical systems.[2] This new structure is considered to be fully-solvated hydrated protons with three-dimensional structure. The result suggests that surface-bound hydrated protons may be important intermediates in the electrochemical interconversion between atomic hydrogen adsorbates and solvated protons in the bulk phase.Reference[1]W. Schmickler, Interfacial Electrochemistry, Oxford, New York, 1996. [2]Kim, Y.; Shin, S.; Kang, H., Zundel-like and Eigen-like Hydrated Protons on a Platinum Surface. Angew. Chem. Inter. Ed. 2015, 54, 7626-7630.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-189**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Temperature dependent carrier dynamics of cesium lead bromide perovskite single crystals

박철우 YIN WENPING 차지현[1] 정덕영[1] 안태규[*]

성균관대학교 에너지과학과 [1]성균관대학교 화학과

Organic Inorganic hybrid perovskite such as MAPbX3 and FAPbX3 (MA=methyl amine, FA=formic amine, X = I, Br, Cl) is widely applied to various devices due to unique properties of tunable band gaps and cost-effective fabrication process. However it has the short-term stability under ambient condition. To overcome the long-term stability, researchers used cesium cation instead of MA. Still inorganic cesium perovskite needs to characterize its optical properties to apply for solar cell applications. Therefore, we monitored that temperature dependent charge carrier kinetics of cesium lead bromide (CsPbBr3) using time-resolved photoluminescence. We report two photoluminescence spectra of free exciton and bound exciton recombination with a temperature increase from 77K to 290K. Our results show the two discrete photoluminescence lifetimes due to the recombination processes and PL intensity ratios for an inorganic perovskite cesium lead bromide single crystals.

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장소: 일산 KINTEX
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발표분야: 물리화학
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Single Molecule Microscopy of Spatially Heterogeneous Dynamics in Supercooled 1,3,5-Tris(naphthyl)benzene

이수현 팽기욱*

성균관대학교 화학과

Amorphous systems lacking long range order in the temperature range between the melting temperature, T_m, and the glass transition temperature, T_g, are known as supercooled liquids. They remain one of the least understood types of condensed matter; therefore, their fundamental properties as well as applications are of interest. Supercooled liquids exhibit nonexponential relaxations and are believed to have sub-micron sized regions of molecules exhibiting relaxation times that can differ by orders of magnitude from these in neighboring regions. To observe the length scales over which these heterogeneous regions exist and the time scales on which they persist while avoiding ensemble averaging over multiple regions, a single molecule (SM) approach becomes crucial. SM fluorophores embedded in the glass former host are believed to mimic the dynamics of its surrounding molecules. By observing many individual probes' rotational relaxation rates simultaneously using wide field single molecule microscopy across temperatures near T_g, the dynamics of the supercooled liquid can be monitored. The breadth of rotational relaxation times will report on the spatial heterogeneity of the system while the changes in a particular probe's dynamics over time reports on temporal heterogeneity, i.e. whether the dynamics are changing from fast to slow or vice versa.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **PHYS.P-191**

발표분야: 물리화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Reduced Dimensional Umbrella Sampling (RDUS) Technique: A General and Efficient Way of Determining Free Energy Surfaces of Complex Reaction Coordinates

백용수 최철호*

경북대학교 화학과

Reduced dimensional umbrella sampling (RDUS) has been introduced to describe the Gibbs free energy surface of multi-dimensional reaction paths. It is a simple and efficient method to reduce multidimensional space by sampling along the reaction path between the reactant and product internal modes. The RDUS technique has been applied to two multidimensional reactions; double proton transfer of acetic acid dimer and hydrolysis of methyl diazonium ion. Gibbs free energy surfaces of those reaction paths have been examined by quantum mechanics/molecular mechanics molecular dynamics (QM/MM-MD) in combination with RDUS technique. It has been proved that the RDUS technique effectively demonstrated the free energy surface of those reactions with one-dimensional reaction coordinate.

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II-VI Colloidal Nanoplatelet Synthesis by Cation Exchange

정주연 김주형 정광섭*

고려대학교 화학과

Colloidal nanoplatelets (NPLs) have been of great interest for the last decade due to its peculiar optical and electrical properties. By varying the thickness of the NPL, the electronic transition swiftly changes depending on the degree of quantum confinement effect. Interestingly, the NPLs with narrow bandgap have not been thoroughly investigated although the exciton created in the narrow-bandgap NPLs can offer invaluable information to us for understanding the performance of optoelectronics. Here, we present the cation-exchanged II-VI NPLs showing dramatic shift of electronic transition wavelength from visible to infrared regime. The gradual quenching of the visible electronic transition and the rising of the narrow-bandgap NPLs are both monitored. The cation-exchange will be a great option to synthesize a narrow-bandgap NPLs that cannot be directly synthesized.

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발표분야: 물리화학
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Time and space resolved LIF detection of OH radical generated by interface electrical discharge

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Most of the energy is generated by combustion of fossil fuel, but the problem of combustion of fossil fuel is that it produces pollutants. A OH radical can be used to solve this problem, because the OH radical has high reactivity. For this reason, the purpose of this experiment is to find the optimum conditions of production of OH radicals by using a discharge. In this study, hydrogen gas is applied on the electrode. A voltage of electrode is about 8.8 kV. The electrode is consisted of two part, one of them is a 1/8 inch stainless steel tube. This tube generates discharge and supplies hydrogen gas. A distance between two parts of the electrode is about 0.5 cm and laser passes between them. The OH radical is detected by using laser-induced fluorescence (LIF). Nd:YAG Laser (NY 61, Continum) was used to pump a dye laser (ND 60, Continum), which excites the OH radical $v'=1 \leftarrow v''=0$ at 283 nm using Rhodamine 6G. Although $v'=0 \leftarrow v''=0$ transition has a high intensity, we used the $v'=1 \leftarrow v''=0$ transition because we already have 300 nm long pass filter. Four mirrors reflect 280 nm – 300 nm and 350 mm focus lense to reduce a laser spot. Because the electrode is attached to rail carrier and lab jack, a position and a height of the electrode can be changed. We measured changes of OH radical when the distance of electrode changes. A position of PMT and laser path are fixed. The change of OH radical is measured by moving the position of the electrode. Also we can change a delay by delay generator to detect a OH radical after discharge. The time for discharge is about 10 ms, we can detect the change of OH radical by observing changed LIF intensity.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **PHYS.P-194**
발표분야: 물리화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Characterization of Human serum albumin–amyloid-β Complex Using Multiple Biophysical Approaches

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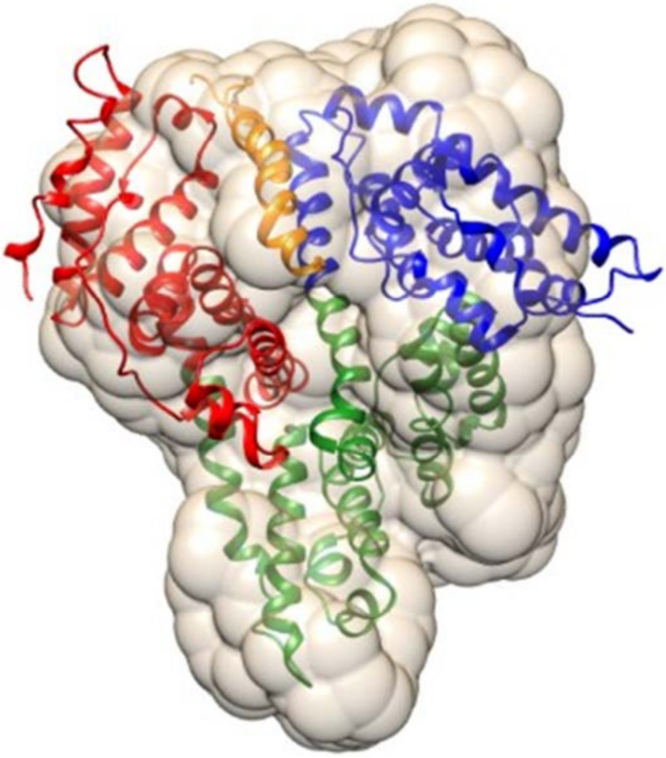
POSTECH 화학과 [1]고려대학교 화학과

Amyloid-β peptide 40 (Aβ40) and 42 (Aβ42) form β-sheet rich, long amyloid fibril that is linked to Alzheimer's disease (AD). The molecular mechanism of Aβ fibrillation has been widely investigated to understand the progress of AD. Then, recent studies have developed a rational strategy for suppressing the fibrillation of Aβ peptides. Human serum albumin (HSA), the most abundant protein in human serum and cerebrospinal fluid (CSF), forms a complex with Aβ peptides, and inhibits fibril formation of Aβ peptides. Thus, the understanding of HSA–Aβ complexation is crucial to the development of the rational strategy for the fibril suppression. In this poster presentation, we will discuss the interaction between HSA and Aβ40 & Aβ42 peptides using various biophysical approaches (mass spectrometry, small-angle X-ray scattering, circular dichroism spectroscopy, and molecular dynamics simulation).



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-170**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Single Particle Study on Size-dependent Optical Properties of Gold Nanospheres beyond the Quasi-Static Limit

서민정 하지원* 김근완 이소영

울산대학교 화학과

Gustav Mie solved Maxwell’s equations to account for the absorption and scattering of spherical plasmonic particles in 1908. Since then much efforts have been devoted to the size dependent optical properties of gold nanoparticles. However, our understanding of the dark-field (DF) scattering properties of single gold nanospheres (AuNSs) beyond the quasi-static limit is still limited, and there have been no studies to elucidate their optical properties under differential interference contrast (DIC) microscopy. We therefore employed single particle DF and DIC microscopy to investigate the particle size dependency for AuNSs with different diameters from 100 nm to 400 nm beyond the quasi-static limit. We found that higher order plasmon resonances are observed in the single particle scattering spectra of large AuNSs (300 nm and 400 nm). Furthermore, the DF and DIC intensities were linearly increased as the particle size was varied from 100 nm to 400 nm. Therefore, the results provide useful experimental information about how the optical properties evolve with the particle size for designing the optimal plasmonic AuNSs or nanostructures in a particular use.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-171**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Characterizing the Optical Properties of Single Gold bipyramids with Sharp Tips as Single Particle Orientation Probes

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Plasmonics metallic nanoparticles have a potential for various applications in optics, catalysis, sensor, medicine etc. Recently, single metallic nanoparticles are gaining much attention as an attractive biomolecular sensor. Especially, gold bipyramids are expected to be a promising material for biosensors to obtain high detection sensitivity due to its sharper tips compared with spherical gold nanoparticle or rod-shape gold nanoparticle and present high scattering cross-section. Herein, we performed single particle study to characterize the optical properties of gold bipyramids with sharp tips under scattering-based dark-field (DF) and differential interference contrast (DIC) microscopy, and to examine their use as orientation probes in biological and physical studies. We found polarization-dependent DIC images and intensities of single gold bipyramids, which enabled for the determination of their orientation angle under DIC microscopy. Furthermore, we found that DIC polarization anisotropy can be obtained from the orthogonally polarized bright and dark intensities for more accurate and reliable angle measurements of single gold bipyramids.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-172**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Three-dimensional Defocused Orientation Sensing of Single Bimetallic Core-Shell Gold Nanorods as Multifunctional Optical Probes

문성우 하지원* 김근완 이소영

울산대학교 화학과

Bimetallic core-shell gold nanorods (AuNRs) are promising multifunctional orientation probes that can be employed in biological and physical studies. This paper presents the optical properties of single AuNRs coated with palladium (Pd) and platinum (Pt) under scattering-based dark-field (DF) microscopy. Strong longitudinal plasmon damping was observed for the bimetallic AuNRs due to Pd and Pt metals on the AuNR surface. Despite the strong plasmon damping, the bimetallic AuNRs yielded characteristic doughnut-shaped scattering patterns under defocused DF microscopy. Interestingly, a solid bright spot appeared at the center of the defocused scattering patterns due to strong damping in the longitudinal plasmon and the increased contribution from the transverse dipoles to the image patterns, which was verified further by a simulation study. Furthermore, the defocused scattering field distributions enabled a determination of the three-dimensional (3D) orientations of single bimetallic AuNRs through a pattern-match analysis technique without angular degeneracy. Therefore, deeper insight into the optical properties and defocused scattering patterns of single bimetallic AuNRs is provided, which can be used to develop multifunctional optical probes that are capable of sensing of the 3D orientation of a probe, biomolecules based on LSPR shift, gas and humidity, etc.

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장소: 일산 KINTEX
발표코드: **ANAL.P-173**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Direct Screening of H7N9 Virus DNA based on Spectral Imaging without Target Amplification

이승아 강성호*

경희대학교 응용화학과

Total internal reflection scattering (TIRS) along with a transmission grating (TG) was effectively utilized for quantitative DAN screening without amplification process. Gold nanopad was used as a substrate for analyzing hybridization of single-stranded DNA (ssDNA)-TIRS nanotag (silver nanoparticles). The TG separated the scattering signals of the nanotag from the substrate and displaced the optical path of the scattered signals to avoid errors caused by several acquisitions, especially for studying plasmonic metal tagged samples (i.e., influenza A; H7N9). This nanobiosensor based on sandwich hybridization quantified the target virus DNA until 74 zM (LOD) without interference of the gold nanopad substrate by using TG. The development is a significant advance in the development of a PCR-free biosensor to greatly reduce the time of sample pretreatment for quantitative screening of influenza A (H7N9) virus.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-174**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Super-Localization of Immunoplasmonic Particle for Ultra-Sensitive Detection of Alpha-Fetoprotein on Nanobiosensor by Scattering-Based Super-Resolution Microscopy

안수진 강성호[1,*]

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Immunoplasmonic particles were super-localized within highly specific region for sensitive detection of alpha-fetoprotein (AFP) with total internal reflection scattering super-resolution microscopy (TIRS-SRM). 20-nm silver nanoparticles were used as a nanoprobe to detect AFP molecules and 100-nm gold nanoisland (GNI, substrate) were selected as a substrate. Individual scattering signals and images of immunoplasmonic particle and GNI were acquired within evanescent field layer by TIRS-SRM using 405 nm and 635 nm illumination, respectively. The center coordinates of the Immunoplasmonic particles were determined within highly specific region (GNI) by applying 2D Gaussian fitting to point spread function. Limit of detection (LOD) of the developed method was 7.04 zM, which was at least 100 times lower than LODs obtained with the previously reports. The TIRS-SRM was demonstrated to be an effective tool to localize individual protein molecules within specific regions for distinguishing each signal and sensitive detection. The method was reliable and effective detection of disease-related protein molecules as diagnostics.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-175**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Immunoreaction-based dual-wavelength capillary electrophoresis for simultaneous detection of thyroid hormones

우나인 강성호[1,*]

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Immunoreaction-based capillary electrophoresis (CE) with a laser-induced fluorescence (LIF) detector was developed for the fast and highly sensitive detection of thyroid hormones. Thyroid hormones have been reported to influence various diseases such as hypothyroid, hyperthyroid, thyroidectomy, and thyroiditis. Therefore, measurements of T4, T3, and TSH are useful for the clinical evaluation of thyroid function. In this study, immunoreaction and biotin-streptavidin interaction were investigated for highly sensitive detection of thyroid hormones as a function of migration time and separation efficiency. Various factors such as the effective length, separation voltage, and pH of running buffer were also examined in order to determine the optimal CE conditions. All three standard thyroid hormones were analyzed within 3.2 min in 25 μM $Na_2B_4O_7$-NaOH buffer (pH 9.3) without losing resolution under optimum conditions, which were 1,000-100,000 times more sensitive than other previous detection methods. In addition, the CE with LIF detection method also successfully applied to the analysis of real human blood samples. Consequently, the immunoreaction-based CE method with LIF detection is an effective, rapid analysis technique for highly sensitive detection of thyroid hormones related to thyroid gland disease.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-176**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Real-Time In-Situ Nano-Carrier Quantification by Super-Resolution Microscopy in Live Single Cells

Chakkarapani Suresh Kumar 강성호[1,*] 신재호[1]

경희대학교 화학과 [1]경희대학교 응용화학과

The extent of time-dependent subdiffraction-limit super-resolution imaging in single molecule tracking and localization has been a great asset in the biomedical field. Quantifying and assessing drug/gene-carrying nanoparticles at the cellular level was crucial in visualizing the nano-toxicity to hold good for drug delivering applications. In this work, a 50 nm drug carrier containing rhodamine B isothiocyanate dye was quantified, tracked, and assessed toxicity at HEK293, NIH3T3, and RAW 264.7 cells using direct stochastic optical reconstruction microscopy (*d*STORM). Results suggest that the RAW 264.7 cells possess higher uptake efficiency of nano-carrier than HEK293 and NIH3T3 cells. Moreover, the nano-carrier was observed to break the biological barrier to be internalized within the nuclei of RAW 264.7 and HEK293 cells. Additionally, the micronuclei were detected more in RAW 264.7 cells than in other two cells suggesting disruption in usual chromosomal DNA breakage. A first ever combined approach of *d*STORM, transcriptomics, and molecular biology paid way for assessing nano-carrier in three different cells at specific sites with precise sensitivity. The subdiffraction-limit super-resolution microscopy *d*STORM resolves quantitative differences in the uptake efficiency of nano-carrier and assess internalized nano-carrier locality in live single cell.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-177**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Detection and optimization of sample preparation of ricin by immunomagnetic separation and liquid chromatography-tandem mass spectrometry

권지현 이용한*

국방과학연구소 5본부 3부

Ricin is a toxic protein derived from castor beans and consist of a cytotoxic A chain and a galactose-binding B chain covalently linked by a disulfide bond, which can inhibit protein synthesis and cause cell death by binding the surface of cell. Due to its high toxicity, ricin has been listed as both chemical and biological warfare agents in Chemical Weapon Convention (CWC). The direct analysis of ricin by mass soectrimetry is not possible because ricin is a ~62kDa protein with a high level of structural heterogeneity. To overcome this limitation is to work on enzymatic digest of the ricin. Our studies were focused on the optimization of sample preparation of ricin. We indroduced the immunomagnetic separation (IMS) method to isolate the ricin from the matrix, allowing the extracted ricin to be further digested and analyzed by liquid chromatography-tandem mass spectrometry (LC-MS/MS). Through this study, the optimized sample preparation was applied to first biotoxin sample analysis proficiency test from the organization for the prohibition chemical weapons (OPCW).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-178**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

NMR study of Arginine ε-NH NMR Signal Assignment in Human Cytosolic Adenylate Kinase 1

김길훈 원호식*

한양대학교 응용화학과

In many of nucleotide binding proteins, Arg residues are known to play important roles in substrate binding through the electrostatic interaction of positive charge on the Arg side chain with the negative charge of phosphoryl group. Adenylate kinase1(AK1) has some Arg residues necessary for binding its substrates, MgATP, AMP. To investigate the interactions between Arg side chains and the substrate in aqueous solution, we observed the signals of Arg ε-NHs of ^{15}N-labeled AK using ^{1}H, ^{15}N two dimensional NMR. The experiments with HSQC pulse sequence detected 13 signals corresponding to all Arg residues on human cytosolic AK1(hAK1). In NMR spectra, we used single quantum coherence SQC as pulse sequence, only the ε-NH signal on Arg side chain can be detected in the specific resonance region. These signals are good markers to study the inter actions between the substrate and proteins with high molecular weight. However, this process is often hard to assign near the terminus of the long side chain such as Arg residues. Therefore, we focused of on six conserved Arg and assigned only these signals by comparison with the spectra of each Arg mutant. The 6 signals derived from 6 Arg residues conserve beyond species (Arg[44], [97], [128], [132], [138], and [149]) were assigned using each mutants which substituted by Ala residue (R44A, R97A, R128A, R132A, R138A and R149A). This method had the problem that the structural perturbation induced by the substitution of amino acid would make the assignment impossible. In the spectra of R44A, R97A, and R128A mutants, there were few problems. Although some perturbations appeared by occurred in R132A, R138A, and R149A of AK1 mutants, the consideration of the assignment for the other signals permitted these signal to be assigned.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-179**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Substrate Binding Studies of Human Cytosolic Adenylate Kinase1 by NMR

김길훈 원호식*

한양대학교 응용화학과

Arginine residues are known to play important roles in substrate binding through the electrostatic interaction of positive charge on the Arg side chain with the negative charge of phosphoryl group in many of nucleotide binding proteins. Human cytosolic adenylate kinase1(hAK1) has some Arg residues necessary for binding its substrates including MgATP and AMP. To investigate the interactions between Arg side chains and the substrate in aqueous solution, we observed the signals of Arg ε-NHs of ^{15}N-labeled AK using ^{1}H, ^{15}N two dimensional NMR. The experiments with SQC pulse sequence detected 13 signals corresponding to all Arg residues on hAK1(human cytosolic AK1). The 6 residue signals (Arg[44], [97], [128], [132], [138], and [149]) playing important roles in substrate binding associated with LID and AMP binding domain out of all corresponding 13 Arg residues were selectively assigned through Arg to Ala substitution. In kinetic studies, the resulting large increases in the $K_{m,app}$ values for AMP^{2-} of the mutant enzymes, the relatively small increases in the $K_{m,app}$ values for $MgATP^{2-}$, and the fact that the R132A, R138A, and R149A mutant enzymes proved to be very poor catalysts are consistent with the idea that the assigned substrate binding sites. Two substrates, MgATP and AMP were titrated into wild type hAK1 and mutants to observe the effects on these assigned signals. The addition of AMP affected 4 Arg signals, whose chemical shift took place a down field in the direction on proton dimension whereas the addition of MgATP did few effects. We were able to find that the Arg[44] specifically interact with the phosphoryl group of AMP. The additions of both the substrates augmented significantly the intensity of Arg[149] signal, which had very low intensity on the spectrum of free wild type AK1. Three ε-NH signals derived from Arg[123], [132], and [138] were broadened and disappeared upon the Mg-ATP addition. These arginine residues locate on α-helix and the following loop along the moiety of triphosphate of MgATP.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-180**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Supersensitive Plasmonic Single Nanoparticle-based Cancer Antigen 125 Immunodetection by Dual-Mode Wavelength-Dependent Enhanced Dark-Field Microscopy

주소영 강성호[1,*]

경희대학교 일반대학원 화학과 [1]경희대학교 응용화학과

A supersensitive immunodetection was achieved for the biomarker cancer antigen 125 (CA125), which was developed based on characterization of single-particle plasmonic scattering by dual-mode wavelength-dependent enhanced dark-field microscopy (EDFM-DM). For simultaneous dual-detection, an electron multiplying cooled charge-coupled device camera and color digital camera were used for qualitative and quantitative analysis, respectively, based on the dark-field scattering images. To prove the efficacy of EDFM-DM for the dectection of scattering signals, various size of different plasmon nanoparticles (i.e., gold nanoparticles, 5 nm, 12 nm, 20 nm, 100 nm and 250 nm; silver nanoparticles, 20 nm, 30 nm, 40 nm, 80 nm and 100 nm) were used as the detection tags and investigated with wavelength dependence of the light source, and the quantum efficiency of the electron-multiplying charge-coupled device camera, 40-nm silver nanoparticle (AgNP) was selected as an optimum fluorescence-free probe. CA125 ovarian cancer antigen was screened at single-molecule level and quantitatively analyzed by measuring the scattering signals of 40-nm AgNP on gold-nanodots arraychip with lowest possible LOD (4 μU/mL, $S/N = 3$) with a wide dynamic detection range of 4 μU/mL-80 U/mL ($R = 0.9935$), which was a 100-375,000-fold lower detection limit with a 100-100,000-fold wider dynamic range than previous detection methods. In addition, recovery was greater than 98% with the spiking of standard CA125 in human serum samples. Dual-mode EDFM-DM based optical property of the plasmon nanoparticle allowed us for a sensitive detection of disease related biomolecules at single-molecule level.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-181**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Platinum-coated Core-Shell Gold Nanorods as Multifunctional Orientation Sensors in Differential Interference Contrast Microscopy

이준호 김근완 하지원*

울산대학교 화학과

We characterized optical properties of single platinum-coated core-shell gold nanorods (Pt-AuNRs) under dark-field (DF) and differential interference contrast (DIC) microscopy. Furthermore, we examined their potential use as multifunctional orientation probes. The longitudinal surface plasmon resonance damping is observed for single Pt-AuNRs due to Pt metals coated on the AuNR surface under single particle scattering spectroscopy. Despite the strong plasmon damping with much decreased scattering intensity, DIC microscopy allowed us to detect single Pt-AuNRs with much higher sensitivity. We found polarization-dependent DIC images and intensities of single Pt-AuNRs, which allows us to determine their orientation angle under DIC microscopy.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-182**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Simultaneous analysis and time-concentration profiles of soman and VX adducts to butyrylcholinesterase and albumin in rhesus monkey plasma by liquid chromatography-tandem mass spectrometry

이진영 권지현 이용한*

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A sensitive method for the purification and determination of two protein adducts, organophosphorus (OP)-BChE and OP-albumin adducts in a single sample of the use simultaneously in the sample preparation step has been developed and validated using liquid chromatography-tandem mass spectrometry (LC-MS/MS). Firstly, we used immunomagnetic separation (IMS) method to isolate the OP-BChE adducts and the HiTrap^{TM} Blue affinity column was followed by used to isolate and purify OP-albumin adducts from the rhesus monkey plasma that was exposed to nerve agents. Also, we studied the time-concentration profiles of two biomarkers, OP-nonapeptides and OP-tyrosines derived from OP-BChE and OP-albumin adducts up to 8 weeks and knew that OP-tyrosines are more favorable biomarkers than OP-nonapeptides due to their long life time. We expect that this intergrated approach will also be used to quantify other types of OP-BChE adducts and OP-albumin adducts in humen plasma, thus serving as a possible general assay for biomarkers of exposure to nerve agents.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-183**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Metabolic alteration induced by IDH1 R132H mutant of glioma revealed by LC-MS/MS

황민지 김민식*

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Glioma is a type of brain tumor originating from tissues that bind and nourish neural tissue inside the brain and spinal cord. Most patients who are diagnosed with glioblastoma, the most common type of glioma have a median survival rate only for about 14 months, and only 3 to 5 percent of the patients are known to survive for more than 5 years [1][2]. Recently the R132H mutation of isocitrate dehydrogenase 1 (IDH1) were discovered in glioblastomas [3]. IDH1 is a metabolic enzyme that catalyzes the oxidative decarboxylation of isocitrate, producing alpha-ketoglutarate in the cytosol [4]. However, the IDH1 R132H mutant enzyme converts isocitrate to 2-hydroxyglutarate (2HG) instead that leads to a hypermethylated state of DNA and histones altering different gene expression in glioma [5]. The goal of this study is to quantitatively survey the metabolic profiles between normal IDH1 and mutant IDH1 R132H by LC-MS/MS. We found that a number of metabolites related to major metabolic pathways were altered with the IDH1 R132H mutation in glioma. This result can be used to find potential targets in glioma with the IDH1 R132H mutation. We expect that the comprehensive understanding of metabolic alteration induced by IDH1 R132H mutant of glioma may help the development of inhibitory drugs that may rectify the altered metabolic pathways by 2HG.

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장소: 일산 KINTEX
발표코드: **ANAL.P-184**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Circulating Biomarker Database (CBD), A Comprehensive Transition Database for LC-MS/MS Based Screening for FDA-approved Biomarkers in Blood

김두영 김민식*

경희대학교 응용화학과

Biomarkers are a type of biological molecules that are objective indications of medical state which can be measured accurately and reproducibly.[1] Currently, there are thousands of biomarker tests approved by FDA and only a few are being measured when a clinical concern is raised by medical doctors. Although the early diagnosis can be done by monitoring them regularly, there is no FDA-approved method to carry out the routine measurement of these biomarkers in a global fashion. Recent advance in high resolution mass spectrometry can now allow a clinical laboratory to measure analytes of interest from specimen very accurately and reproducibly.[2] Especially, the targeted mass spectrometry such as MRM (multiple reaction monitoring) has the potential to be the major technology to monitor these thousands of biomarkers in a clinical setting. In this regards, we create a database called Circulating Biomarker Database (CBD) as the first step which is a comprehensive transition list for LC-MS/MS-based screening of FDA-approved biomarkers. In this database, precursor ions of 583 biomarkers and their fragment ions as transitions are listed together towards a comprehensive monitoring method to screen most biomarkers in blood. In conclusion, Circulating Biomarker Database can be used for clinical diagnostics and prognostics in the future medicine.

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Enhanced quantification of phospholipids using isotope-labeled methylation using nUPLC-ESI-MS/MS

이종철 변슬기 문명희*

연세대학교 화학과

Phospholipid (PL) is one of the most important type among various lipid classes in biological cells. Quantitative analysis of PLs is crucial as they regulate several important functions such as formation of cell membrane, intercellular signaling, and energy storage. Conventionally, lipid quantitation using LC-MS is often carried out with the addition of internal standards to compensate the ionization fluctuation. However, the use of internal standards is limited by several reasons; lipid standards of various molecular structures are limited and accurate determination of lipid amount is difficult. In this study, a quantitative analysis of PLs was accomplished, based on an isotope-labeled methylation (ILM) method using (trimethylsilyl)diazomethane as a methylation reagent to methylate the phosphate or carboxyl group. MeOH and HCl were utilized for light isotope-labeled methylation, while MeOD and DCl containing deuterium were used for counterpart methylation. ILM method was validated concerning efficiency of methylation, optimization of modifiers, and peak area linear relationship of H- and D- labeled methylated lipids. This method consequently applied to DU145 cell line with and without D-allose treatment. In the end, a total of 112 PLs including LPG, PG, LPS, PS, LPA, PA, and CL were identified. Among these lipids, 8 and 25 more PAs and CLs, respectively, were detected from ILM method, when they were not detected in intact lipid extracts.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Top-down proteomic analysis of HDL from coronary artery disease patients using flow field-flow fractionation and mass spectrometry

이재현 양준선 문명희*

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Coronary artery diseases (CAD) refers to a condition in which coronary arteries become narrow by accumulation of cholesterols, fats, and other substances. Narrow arteries restrict blood flow to heart and may even cause a partial or complete blockage of arteries. High-density lipoprotein (HDL) has been reported to be associated with CAD of which few marker proteins are of interests. HDL is composed of various lipids and proteins including apolipoproteins and recent studies have reported that apolipoprotein A-I (apo A-1) in HDL undergoes oxidation during the development of CAD. As other types of proteins in HDL are highly likely to undergo changes, analysis of HDL-related proteins is necessary to understand the relationship between HDL and CAD more effectively. Flow field-flow fractionation (FlFFF) is a separation technique based on size in a range of nano to micrometer and in this study, FlFFF was applied to separate the HDL from human plasma of CAD patients. A miniaturized asymmetrical FlFFF (AF4) channel was coupled on-line to electrospray ionization mass spectrometry (ESI-MS) for a high speed separation of lipoproteins and top-down proteomic analysis in order to investigate the perturbation in HDL-related proteins due to development of CAD.

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Evaluation of risk factors for non-alcoholic fatty liver disease using nanoflow UPLC-ESI-MS/MS

변슬기 문명희*

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Non-alcoholic fatty liver disease (NAFLD) is one of the most frequent cause of deaths worldwide, associated with obesity and insulin resistance due to unhealthy lifestyle. With excessive amount of fat accumulated on liver tissue, a spectrum of NAFLD encompasses a wide range of conditions ranging from simple steatosis to advanced cirrhosis. As a number of factors such as high cholesterol diet and inflammation are possible risk factors of NAFLD, the effect of various risk factors on hepatic lipid metabolism was evaluated in this study using nanoflow ultrahigh-pressure liquid chromatography electrospray-ionization tandem mass spectrometry (nUPLC-ESI-MS/MS). Lipids from hepatic tissue from rabbits grown under the conditions of healthy diet (C), inflammation by injecting carrageenan (I), high cholesterol diet (HC), and high cholesterol diet with inflammation by injecting carrageenan (HCI) were structurally identified based on collision-induced dissociation (CID) spectra obtained from nUPLC coupled with ion trap MS, followed by a targeted quantification of the identified lipids using nUPLC coupled with triple quadrupole MS in selective reaction monitoring (SRM) mode. Over 300 hepatic phospholipids, sphingolipids, and glycerols were analyzed and significant and dramatic changes were observed from HC and HCI groups but not I, indicating that intake of high cholesterol food altered hepatic lipidome significantly while inflammation did not.

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Effect of cationic monomer composition on polymerization of cationic polyacrylamide copolymers using frit-inlet asymmetrical flow field-flow fractionation with multi-angle light scattering

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Cationic polyacrylamide (CPAM) copolymers are often used as flocculants in wastewater treatment and they have high molecular weight distribution (~108 g/mol) and viscosity. Physicochemical properties of CPAM depend on polymerization methods (solution polymerization and emulsion polymerization), chain types (linear and branched), cationic monomer composition, and amount of cross-linking agent. In this study, influence of these factors on molecular weight distribution and conformation of CPAM copolymers was evaluated using an elution-based separation technique, flow field-flow fractionation (FlFFF), and multi-angle light scattering- differential refractive index (MALS-DRI). In terms of cationic monomer composition, CPAM tended to become more compact with increased molecular weight distribution when cationic monomer composition was increased in solution polymerization and in emulsion polymerization, CPAM seemed to be aggregated when cationic monomer composition was less than 10 mol%. When the amount of cross-linking agent was increased, CPAM tended to be synthesized smaller and more compactly. Also, FlFFF is operated in either normal or steric/hyperlayer mode depending on the size of sample particles and in this study, a transition between two different modes of separation was observed under gradient elution.

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발표분야: 분석화학
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Analysis of prostate cancer-derived urinary exosomes by flow field-flow fractionation

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연세대학교 화학과

Exosomes are extracellular vesicles with 20 to 100 nm in diameters and they are involved in intercellular communication by transporting biomolecules such as mRNA, proteins, and lipids. They exist in all kinds of body fluids including urine and blood. Recently, research on exosomes of body fluids has emerged as a crucial component in biomedical field as exosomes are reportedly potential biomarker candidates of many diseases. Among various types of exosomes, urinary exosomes are closely associated with a development of prostate cancer (PCa) and their sizes are different compared to healthy controls. Flow field-flow fractionation (FlFFF) was used in this study to fractionate urinary exosomes by their size. FlFFF is an elution-based method for separating sample components according to size by an increasing order of hydrodynamic diameters and as raw samples can be directly injected into an empty FlFFF channel, the separated sample components can be collected in their intact forms, which is one of a great advantage of using FlFFF. In this study, urinary exosomes from healthy controls and PCa patients, which were first isolated from fresh urine samples by ultracentrifugation, were separated by FlFFF and clear difference in size distribution between two groups was observed. Furthermore, size-separated urinary exosomes were collected for lipidomic analysis using nUPLC-ESI-MS/MS and different lipidomic profiles and variations from large- and small-sized exosomes were observed between the groups.

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

김산하 문명희* 양준선

연세대학교 화학과

Lipoproteins are carrier molecules that transport lipids and cholesterol in the bloodstream. Low levels of high-density lipoprotein (HDL) and high levels of low-density lipoprotein (LDL) in plasma are known to be related with the development of various types of diseases. Therefore, it is important to study lipoproteins at the molecular level to understand its metabolism and relationship to disease progression. Alzheimer's disease is the most common form of dementia worldwide, taking up around seventy percent of dementia cases. A beta-amyloid, a cause of Alzheimer's disease, is a toxic protein that kills brain neurons as its number increases. As a few studies have reported that beta-amyloid accumulates when HDL is low and LDL is high in plasma, a separate profiling of lipids from HDL and LDL is necessary to understand how the lipid metabolism within each class of lipoprotein is altered when Alzheimer's developed.In this study, HDL and LDL from of pooled plasma samples of human controls, patients with mild cognition impairment, and Alzheimer's disease patients were fractionated by asymmetrical flow-field flow fractionation (AF4) and lipids from the collected fractions of HDL and LDL were extracted. Using nanoflow ultrahigh-pressure liquid chromatography-electrospray ionization-tandem mass spectrometry (nUPLC-ESI-MS/MS), the extracted lipids were structurally identified based on collision-induced dissociation for qualitative analysis and the identified lipids are going to be selectively quantified to evaluate the difference between three groups.

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장소: 일산 KINTEX
발표코드: **ANAL.P-191**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Chemical variations at the interface between UO_2 and Zr by high temperature annealing

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한국원자력연구원 원자력화학연구부 [1]한국원자력연구원 원자력연구팀

The temperature-dependent changes of the interface between uranium dioxide and zirconium in UO_2-Zr systems by various annealing were studied using X-ray photoelectron spectroscopy (XPS). The U 4*f* and Zr 3*d* core-level spectra show that the uranium dioxide exists as hyperstoichiometric UO_{2+x} at room temperature and as UO_2 after annealing with zirconium, whereas the zirconium was spontaneously oxidized to ZrO_2 at room temperature and various features such as α-Zr(O), $(U,Zr)O_2$, ZrO_2, and suboxides after annealing with uranium dioxide. Furthermore, we observed that the molten product was composed of α-Zr(O), $(U,Zr)O_2$ and ZrO_2 when a UO_2-Zr sample was fully melted. In this work, we represented the definite study for the variations of the interfacial products in UO_2-Zr systems as a function of temperature.

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NMR Structural studies associated with the mechanism of Syndecan-4 Receptor

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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. Syndecan-4 interacts with various binding partners to increase wound healing, cell invasion and survival, activates focal adhesion and phosphorylates, and regulate cytoplasmic calcium concentration. In addition, the interaction of syndecan-4 with GFRs (growth factor receptors) is a very important factor in cancer progression and is particularly associated with resistance to treatment and therapy in breast cancer.To get a better understanding of the mechanism and function of syndecan-4, it is crucial to investigate its three dimensional structure. Syndecan-4 comprises three major sections: extracellular (ecto-), transmembrane (TM) and cytoplasmic (Cyto-) domains. Syndecans have a very well conserved cytoplasmic region, but the V regions have a distinctive feature for each syndecan family member. The cytoplasmic domain of syndecan-4 consists of 28 amino acids and includes V domain. The binding of PIP2(phosphotidylinositol (4,5)-bisphosphate) 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-). And its structure was investigated by solution/solid-state NMR spectroscopy.

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발표분야: 분석화학
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Construction of diverse home-built solid-state NMR probes for specific purposes

정지호 김지선 김용애*

한국외국어대학교 화학과

The solid-state NMR has been used to investigate insoluble materials in advanced industrial site. It could be applied to a broad range of organic/inorganic nano-materials including polymers and bio-solids including pharmaceutical drugs and membrane proteins. Solid-state NMR spectroscopy is very valuable to study the structure and dynamics of membrane proteins even though most biological samples on lipid bilayers have high dielectric property due to containing large amounts of lipids, water and salts. We try to make the specific probe with high efficiency and durability for biological samples. Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore(WB) & narrow bore(NB) 1H-15N solid-state NMR probe and a home-built 800 MHz 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 batterypack samples. These two probes provide high efficiency and good RF homogeneity.

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발표분야: 분석화학
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The structural characterization of disease related human transmembrane proteins using the NMR spectroscopy

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Transmembrane proteins play critical roles in biological processes such as 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 transmembrane domain from human amyloid beta protein (hAβ-TM) and second transmembrane domain from human melanocortin-4 receptor (hMC4R-TM2). The hAβ-TM shows membrane-bound oligomeric state, and the Ca2+-permeable ion channel formation of non-fibrillar state in the cell membrane. So these channels can disrupt the normal cellular calcium homeostasis. It causes 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 hAβ-TM and hMC4R-TM2. 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 was successfully obtained by using these solid-state NMR probe.

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일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **ANAL.P-195**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

3D topological studies of antimicrobial peptides with enhanced activities derived from Lactophoricin

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Since wide spread of antibiotic resistance bacterial pathogens have been prevalent it is important to investigate 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 of 11 were designed and modified to enhance antibacterial activity using conservative sequence change. Three peptides were selected among LPcin analogs via results of bacterial killing and growth inhibition assays. 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. 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. And we will also present the optimized design, construction, and good efficiency of a home-built 800 MHz (NB) narrow-bore 1H-15N solid-state NMR probe for solid-state NMR studies of antimicrobial peptides.

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발표분야: 분석화학
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Theoretical calculation of collision cross section for ions in nitrogen buffer gas

고태원 김준곤*

고려대학교 화학과

In ion mobility spectrometry (IMS), repeated collisions between gas-phase ions and neutral buffer gas molecules occur under weak and uniform electric field. The collisions affect ion mobility, which is directly related to ion collision cross section (CCS). CCS is related to ion structure, and different structural isomers show different CCS to be separated during IMS. Then, ion structures can be revealed based on theoretical tools for calculating ion CCS. Accurate description of intermolecular interactions between gas-phase ions and neutral buffer gas molecules is a key factor in estimating theoretical CCS of ions. Nitrogen is a popular neutral buffer gas for IMS and is a linear molecule with quadrupole moment and a large polarizability. Thus, the use of nitrogen as the buffer gas in IMS allows separation of ions with similar structures but distinct dipole moments, which is typically not possible with other drift gases such as helium. At the same time, however, the complexity of the nitrogen gas makes it difficult to develop an accurate theoretical tool for calculating the CCS of ions in nitrogen. Here we present a more accurate calculation method for calculating ion CCS in nitrogen drift gas that are comparable with experimental results. We investigate the influence of van der Waals, ion-induced dipole, and ion-quadrupole interactions on theoretical CCS and optimize these interactions to reduce the error between experimental and theoretical CCS. Through these experiments and calculations, it becomes possible to obtain a more valid and powerful theoretical calculation method.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-197**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Stability of N-glycans Found in Human Saliva using Nano LC Chip/Q-TOF MS

김범진 문한태 안현주*

충남대학교 분석과학기술대학원

For the past decades, saliva glycans hold the attention as a potential bio-signature in clinical and forensic field owing to its inherent advantages; easy access, simple storage, and non-invasive collection. Glycosylation, one of the most common PTMs, plays an important role in a wide range of biological processes. Saliva glycosylation could be altered in the physiological and pathological situations by diseases, external environment, and chemical materials. Although profiling of glycans in saliva for the discovery of potential biomarkers for inflammatory diseases and cancers has been actively performed, fundamental studies such as saliva stability and glycans variations between individuals have been rarely done. In this study, we have investigated variations of saliva N-glycans 1) between individuals (n=18), 2) by a single individual using saliva collected on different days (0, 1, 7, and 30 days), and 3) during the storage of saliva (0, 1, 2, 3, and 7 days) in room temperature. Saliva N-glycans were enzymatically released by PNGase F and then purified and enriched by PGC-SPE. Saliva N-glycans were fully characterized by nano LC chip/Q-TOF MS and MS/MS. Inter- and intra-individual and environmental variations were qualitatively and quantitatively examined through glycan compositions and abundances. This study may help design the experiments and evaluate the saliva glycan candidates for biomarker study.

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장소: 일산 KINTEX
발표코드: **ANAL.P-198**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Characterization of Glycan Signatures of Human Saliva using Nano LC Chip/Q-TOF MS

문한태 김범진 안현주*

충남대학교 분석과학기술대학원

In recent years, saliva has been received attention in forensic field. Saliva encountered at crime scene is one of the most significant evidence and thus, the identification and differentiation of saliva from other human and non-human fluids is an essential prerequisite prior to further crime investigation. However, conventional methods including enzymatic and chemical amylase test to determine saliva have lack of specificity due to cross-reactivity with other fluids. Glycoproteins are the major components of human saliva. Therefore, glycosylation in saliva can be used as a potential candidate of signature of human saliva. Herein, we have explored the possibility of nano-LC/MS-based glycomic approach to identify and differentiate bio-signature between human saliva and other fluids. Briefly, N-glycans in human saliva (7 males and 11 females) were enzymatically released and enriched by PGC-SPE. Human saliva N-glycans were profiled by nano LC-PGC chip/Q-TOF MS and –MS/MS. Saliva N-glycans displayed a heterogeneous mixture of neutral and acidic components and the most of them were decorated with fucose (> 50%). Interestingly, highly fucosylated glycans containing from tetra to octa fucose ($Hex_{5\text{-}7}HexNAc_{4\text{-}6}Fuc_{4\text{-}8}$) were observed in high abundance in human saliva. To explore human saliva-specific glycans, human saliva was compared with other fluids such as human serum, human milk, and animal saliva (rat and bovine) we conclusively determined that highly fucosylated N-glycans were saliva-specific molecules found in only human saliva. Of them tetra fucosylated bi-antennary ($Hex_5HexNAc_4Fuc_4$) and tri-antennary ($Hex_6HexNAc_5Fuc_4$) glycans were present in all human saliva.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-199**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High-throughput Screening of Native Glycans on Therapeutic Glycoproteins using Liquid Handling System

박경미 안현주*

충남대학교 분석과학기술대학원

Glycosylation of biotherapeutics is critically associated with the stability, biological activity, half-life, and safety of drug. The glycosylation could be changed by production environment such as host cell system and culture conditions. Therefore, monitoring the glycosylation at each stage of manufacture process is a suitable approach to assess production quality for drugs. Automative high-throughput tools are currently developed and innovated to treat a large number of samples in a short time span and get high quality data by minimization of hands-on time. Here we have developed the automated analytical platform to enrich and fractionate native glycans using liquid handling system combined with 96-well microplate for a high-throughput manner. Human IgG used as a motif of therapeutic mAbs, a well known glycoprotein, was chosen to develop sample preparation procedure. Overall processes including protein denaturation by heating block, N-glycan release by PNGase F, and glycan purification and enrichment by solid phase extraction have been streamlined and optimized. Glycans were profiled by nanoLC chip/Q-TOF MS. We found total 24 glycans consisting of complex/hybrid type N-glycans w/wo sialic acid residues in both automated and manual treatment. The CVs of normalized peak intensities of top 10 N-glycans were less than 8.2 %, which indicates high comparability between two methods. Moreover, we validated the quantitative reproducibility for 5 different well positions in the 96-well plate. Two independent replicates experiments were performed per day. The Pearson correlation coefficient R between all samples was determined to be above 0.9. Glycan preparation using the automated platform showed to be rapid, reproducible, and reliable and it can be applied for real therapeutic glycoproteins.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-200**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Assessing Biosimilarity of Therapeutic Glycoprotein using Intact Glycopeptide

서영숙 안현주*

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Therapeutic glycoprotein exhibits structural heterogeneity and complexity due to co-occurred glycans on a protein. Drug's glycosylation has enormous effect on biological activity, immunogeneicity, and serum half-life. Therefore, glycomic characterization is of great importance to prove drug's quality. With the increase of biosimilars, analytical tools for glycan profiling have been developed to evaluate the compatibility with the reference drug in efficacy and safety. Here, we present an analytical strategy to determine glycosylation similarity of therapeutic glycoproteins using intact glycopeptide. As a proof of concept, we selected recombinant erythropoietins (rhEPOs) having multiple glycosylation sites and glycan variants. The rhEPO was treated using specific protease, trypsin, to obtain glycopeptides having sugar moieties with peptide tag. We determined two intact glycopeptides of rhEPO in LC/MS analysis. One is major glycopeptide containing two N-glycosylation sites (83Asn and 88Asn), which indicates a distinctive glycosylation pattern with different O-acetylation on NeuAc. The other glycopeptide having three N-glycosylation sites (38Asn, 30Asn, and 25Asn) was also identified by glycan correlation. Using intact glycopeptide analysis, we could rapidly screen the glycoform distribution of rhEPOs for assessing biosimilarity.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-201**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Optical Properties of Urchin-Shaped Gold Nanoparticles under Single Particle Spectroscopy

김근완 하지원*

울산대학교 화학과

Plasmonic gold nanoparticles have received much attention because of their unique size- and shape-dependent optical properties induced by localized surface plasmon resonance (LSPR) effect. In this study, we investigated the optical properties of urchin-shaped gold nanoparticles with sharp and short tips on their surface under single particle microscopy and spectroscopy. We employed scattering-based dark-field (DF) and differential interference contrast (DIC) microscopy to elucidate the optical properties of gold nanourchins (AuNUs) at the single particle level. First, we found that the LSPR peak is redshifted for single AuNUs with sharp spikes on their surface in comparison to spherical gold nanoparticles with same size. Second, we obtained the defocused images of single AuNUs under DF microscopy, which provided three-dimensional (3D) spatial scattering field distributions. Last, we found polarization-dependent DIC images and intensities of single AuNUs under interference-based DIC microscopy, which was not observed for gold nanospheres without sharp tips. Therefore, the results allow us to have a better understanding of the optical properties of single AuNUs with the spiked surface.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-202**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Evaluation of Laser-Induced Breakdown Spectroscopy as a simple method for identifying geographical origins of agricultural products

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한양대학교 화학과

Fast identification of geographical origins of agricultural products becomes more demanding recently. For this purpose, Raman and near-infrared (NIR) spectroscopy have been widely employed since the corresponding measurements are fast and non-destructive with minimal or no sample pretreatments. These spectroscopic methods provides molecular structural information of sample components for the identification; while, the difference in atomic composition in samples is alternatively valuable in many cases. Therefore, laser-induced breakdown spectroscopy (LIBS), which can provide information on almost all elements, has gained an attention. LIBS-based measurement is also fast as nearly non-destructive as comparable with Raman and NIR spectroscopy. Here, we have utilized LIBS for the identification of geographical origin of milk vetch root. The pellets made from domestic and imported milk vetch root samples were measured and the acquired LIBS spectra were used for the discrimination using several chemometric methods. For the collection of representative spectra, LIBS spectra acquired at different spots on each pellet were averaged. The resulting discrimination accuracy was evaluated in conjunction with the difference in the composition of elements.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-203**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Plasmon-enhanced photoluminescence immunoassay for Influenza virus sensing by using gold nanoparticle decorated carbon nanotube

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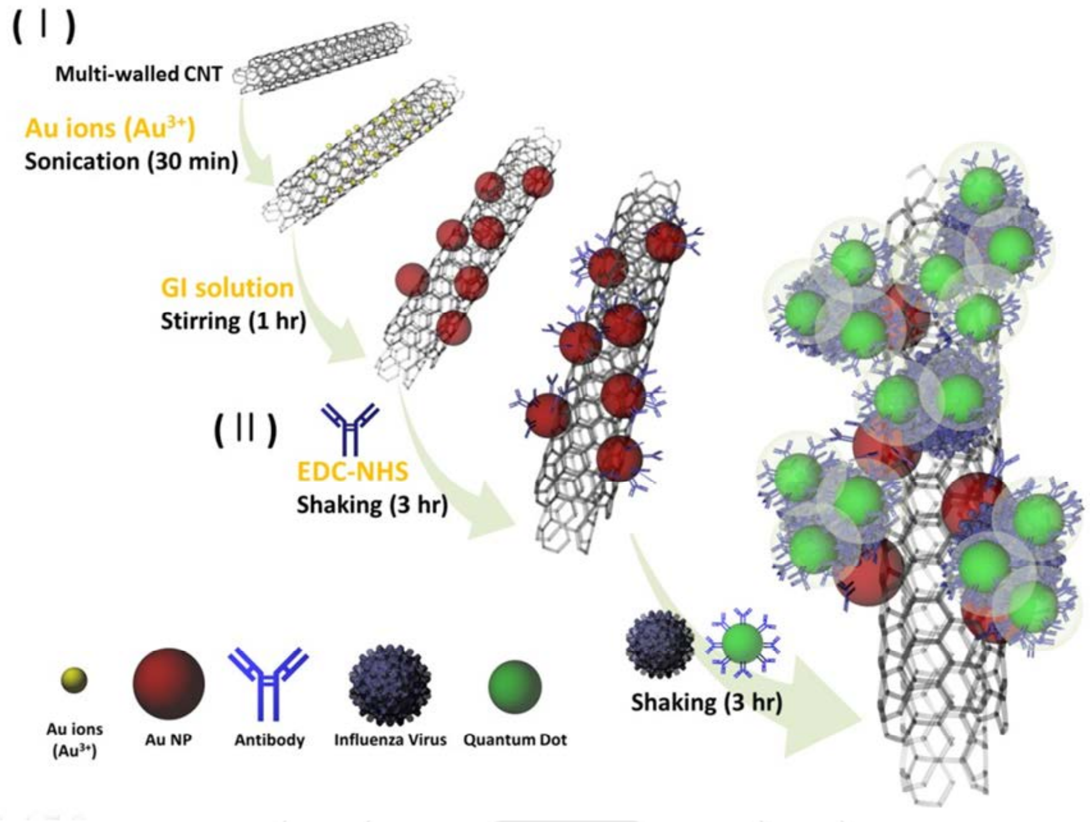
부산대학교 인지메카트로닉스공학과 [1]부산대학교 인지메카트로닉스 공학과 [2]부산대학교 광메카트로닉스공학과

A plasmon-assisted fluoro-immunoassay (PAFI) was developed for the detection of the influenza virus by using Au nanoparticle (Au NP)-decorated carbon nanotubes (AuCNTs) that were synthesized using phytochemical composites at room temperature in deionized water. Specific antibodies (Abs) against the influenza virus were conjugated onto the surface of AuCNTs and cadmium telluride quantum dots (QDs), which had a photoluminescence intensity that varied as a function of virus concentration and a detection limit of 0.1 pg/mL for all three types of influenza viruses examined. The clinically isolated influenza viruses (A/Yokohama/110/2009 (H3N2)) were detected in the range of 50–10,000 PFU/mL, with a detection limit of 50 PFU/mL. From a series of proof-of-concept and clinical experiments, the developed PAFI biosensing system provided robust signal production and enhancement, as well as an excellent selectivity and sensitivity for influenza viruses. This nanoparticle-based technique could be potentially developed as an efficient detection platform for the influenza virus.


(Ⅰ)
Multi-walled CNT
Au ions (Au3+)
Sonication (30 min)
GI solution
Stirring (1 hr)
(Ⅱ)
EDC-NHS
Shaking (3 hr)
Shaking (3 hr)
Au ions (Au3+)
Au NP
Antibody
Influenza Virus
Quantum Dot

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-204**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A Sandwich-type HIV-1 p24 immunoassay using ICP-MS with metal-doped nanoparticles

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단국대학교 화학과 [1](주)에스엘에스 유전체의학연구소

A virus is a type of non-cellular infectious agent that replicates inside the host cells of other organisms. Human Immunodeficiency Virus (HIV) causes acquired immunodeficiency syndrome (AIDS) and HIV-1 p24, a component of the HIV particle capsid, is an antigen detected in infected patients' blood. For detection of HIV-1 p24, the sandwich-type conjugates employing metal-doped magnetic nanoparticles (MNPs) and metal/dye-doped silica nanoparticles (SNPs) were produced by immunoreaction and the concentration of the target was determined by ICP-MS in this work. For this, both Cs-doped Fe_3O_4 MNPs and Gd/RhBITC-doped SNPs for target extraction and tagging as a probe, respectively, were synthesized and immobilized with the antibodies of HIV-1 p24. Feasibility of quantification was shown from the calibration curve plotted the intensity ratio of Gd/Cs vs. the concentration of target. For future work, this method will be applied to real samples and multiplex detection of other viruses.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-205**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Microwave-assisted week acid hydrolysis of proteins using hydrochloric acid generating serial detachment of amino acids

백지현 김정권*

충남대학교 화학과

Microwave-assisted week acid hydrolysis of proteins has been developed as an alternative approach for protein sequence analysis. Microwave-assisted weak acid hydrolysis of proteins can be performed with a small amount weak acid (e.g. 2%) such as formic acid, acetic acid or phosphoric acid in a microwave oven for an hour incubation. Weak acid hydrolysis cleaves exclusively C-terminal of aspartic acid. This method is simpler and faster than using a protease such as trypsin. It was reported that 3 M HCl hydrolyzed a protein into polypeptide ladders with varying sizes of up to molecular mass of the protein. Here we tried to truncate N-terminal of aspartic acid with small amount of hydrochloric acid for microwave-assisted acid hydrolysis after microwave-assisted week acid hydrolysis of myoglobin. The 0.5 ~ 1% HCl hydrolysis of C-terminal truncated myoglobin peptides provided major peptides cleaved selectively at the N-terminal of aspartic acids. The cleaved peptides was identified by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry, where the peptides cleaved with the N-terminal of aspartic acid were observed as major peaks while the peptides with the C-terminal cleavage of aspartic acid were observed as minor peaks.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-206**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Auto-flame synthesis of $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ as cathode materials for Li-ion battery

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울산대학교 화학과

A simple, rapid, and efficient flame synthesis method was developed cathode materials for Li-ion batteries. Therefore, the combustion of the metal nitrate precursors with flame was used to complete synthesis of $LiNi_{0.95-x}Co_xTi_{0.05}O_2$. The complete procedure to achieve the $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ precursor powder was taken under 1 hr. X-ray diffraction (XRD) patterns confirm the formation of single phase of the $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ at 800℃ for 12hr. SEM and TEM analyses show the presence of ultrafine nature of the particles. The fabricated materials show the discharge specific capacity of 159 mAh g^{-1} and 137 mAh g^{-1} at 0.1 C-rate for the initial cycle for the $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ of x = 0.25 and 0.30, respectively. The results indicate that $LiNi_{0.95-x}Co_xTi_{0.05}O_2$ synthesized with environmental friendly route shows a promising electrochemical activity.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-207**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Excellent electrochemical performance and wide operating voltage of phosphate-borate hybrid cathode material for Li-ion battery

지민수 이영일*

울산대학교 화학과

Olivine $LiMPO_4$ (M=Fe, Mn, Co, Ni, etc.) based cathode materials for lithium ion battery widely investigated for electric vehicles and electronic device due to low cost, safety and structural stability. This work reports for the first time lithium iron phosphate and lithium iron borate as a hybrid cathode material. The material has been synthesized without using external carbon source to improve specific discharge capacity with wide operating voltage range. $LiFe(PO_4)_{0.5}(BO_3)_{0.5}$ exhibits a remarkably high specific discharge capacity near the theoretical capacity (97.3%) of 189.8 mAh g^{-1} at 0.1 C. X-ray diffraction and NMR spectroscopy of the pristine material revealed mixed phase of olivine and vonsenite structures. The electrochemical performance of the $LiFe(PO_4)_{0.5}(BO_3)_{0.5}$ showed also polymorphism with two different structured materials. The LFBP cathode material can meet the requirements for high power applications, such as electric vehicles and energy storage for smart grids in the near future.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-208**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Detection and counting of red blood cells via electrochemical collision event on an Ultramicroelectrode

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Information about blood tests is very necessary for diagnosing and detecting blood disorders. Here, we have developed the electrochemical detection of red blood cells (RBCs) using single particle collision events. The staircase current decrease was caused by collision, and gave quantitative information about the size, and concentration of RBCs. The signals obtained by chronoamperometry (CA) measurement during a collision of RBCs with ultramicroelectrode (UME) at the different of RBCs concentration showed high sensitivity and will be essential in the future.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-209**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Detection of water/oil nanoemulsion droplet using electrochemical collisions on an Ultramicroelectrode

HOANGTHITUYETNHUNG HOLETHYTHY 박준희[1,*] 김병권[*]

숙명여자대학교 화학과 [1]전북대학교 화학교육과

Herein, for the first time, research on water/oil emulsion droplet by electrochemical analysis has been reported. By the use of blocking of the single emulsion droplet, water/1,2-dichloroethane emulsion droplets collided with an ultramicroelectrode (UME) leading to the “stair-case” current decrease. Each “stair-case” current decrease corresponds to the emulsion droplet collision on UME surface. The experimental collision frequency is proportional to the concentration of emulsion droplet. In addition, each water droplet size was estimated from the magnitude of the “stair-case” current decrease with simulation data. Results obtained from the collision signals provide information about the single droplet size (nano- to micro-) and a pM concentration of the water emulsion in organic continuous phase.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-210**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Using Electromembrane Extraction for Determination of NSAIDs by HPLC-UV

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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 four Non-steroidal anti-inflammatory drugs(NSAIDs) in human urine samples. The parameters such as pH of acceptor, stirring speed, voltage, support liquid membrane(SLM), and extraction time were optimized. Simultaneous chromatographic separation of four 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 30:70 and after 5minutes, compositon is changed to 15:85, finally, changed to 5:95 after 5minutes. After the extraction, 5 ㎕ of extract was directly injected into the HPLC-UV system.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-211**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Shotgun proteomics-based global proteome analysis of colon cancer cell line from two-and three-dimensional cell culture

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Two-dimensional (2D) cell culture system is well established strategy to perform in vitro cell-based studies regarding to unearthing biological functions of proteins and metabolites in a cell, as well as, in particular, drug(s) screening for cancer cells. Even though 2D cell culture has been considered as a fundamental way to cell-based in vitro studies, it has been, unfortunately, reported that the results concerning both cytotoxicity and activity of drug on 2D cell culture are not fully matched with that of in vivo tissues. Very recently, various strategies for three-dimensional (3D) cell culture have been developed by means of matrix-based or matrix-free platforms, so as to mimic in vivo environment of cells. Based on recent study on 3D cell culture, 3D-cultured cells in morphology, gene/protein expression and drug sensitivity are quite different from that of 2D-cultured cells. In this study, we analyzed the cellular proteome from 2D-cultured colon cancer cell line SW480 and 3D cultured one, thereby profiling the proteome difference according to 2D/3D culture conditions. To do so, we performed a comprehensive proteomic analysis of 2D- and 3D-cultured cells using 2D-nanoLC-ESI-MS/MS experiments. Furthermore, the quantitative assessment of cellular proteome from 2D-/3D-cultured cells also was carried out by using isobaric tags for relative and absolute quantitation (iTRAQ) labeling. Based on our experiment, we found that a number of proteins identified in common from both of 2D-/3D-cultured SW480 are shown to be significantly different between two different culture platforms. From doing this proteomic analysis of 3D-culutred cell line, it allows to be boosted up in discovery of drug that is effective against diverse cancer.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-212**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Feasibility of a compact low-cost laser-induced breakdown spectroscopy device for quantitative analysis of metallic elements in edible salt products

김향 남상호 이용훈*

목포대학교 화학과

We investigated feasibility of a compact low-cost laser-induced breakdown spectroscopy (LIBS) device for quantitative analysis of Ca and Mg in edible salts. By using a compact low-power diode-pumped solid-state (DPSS) laser and a miniature non-gateable charge-coupled device (CCD) spectrometer, the LIBS spectrometer could be significantly simplified. The standard materials were prepared using mixtures of NaCl, $MgSO_4$, and $CaCO_3$ in forms of solid pellets. The DPSS laser beam (270 microjoule/pulse) was focused on the pellet surface through an objective lens. Optical emission from the laser-induced plasma was collected and sent to the non-gateable miniature CCD spectrometer. For each concentration of Ca or Mg, the averaged emission line intensity from the measurements for multiple pellets provided the improved analysis precision in comparison with that obtained from multiple line scans for a single pellet. This indicates that the chemical composition was homogeneous enough and however the measurement condition was not consistent among the multiple line scans within the same pellet. The fluctuation could be averaged out by taking data from multiple pellets. We applied this device and analysis methology to real salt products and discussed its feasibility as a portable in-situ analysis device for salt products.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-213**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication and Application of the Microfluidic Devices Designed to Simulate HET-CAM Test

Tian Tian 조수진 이석우*

공주대학교 화학과

In this presentation, we will describe the development and application of a simple microfluidic device for in vitro irritation tests of cosmetics. The device was fabricated with a three-compartment diffusion system to mimic the HET-CAM system. HUVEC (Human Umbilical Vein Endothelial Cells) was cultured in the three compartments and the tested substances were injected to the reservoir and diffused through the tiny microfluidic channels. The viability of cells in each compartment was monitored by an optical microscope. The IS (irritation score) values were evaluated based on the viability of cells as a function of time when the cells were exposed to the tested substances. Three kinds of cosmetic materials were tested with microfluidic systems, and the results were compared with those of the HET-CAM test to validate the in vitro irritation test system.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-214**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrochemical Detection of Hydrazine Using Poly(dopamine)-Modified Electrodes

NGUYENTHITRUCLY 박준희[1,*] 김병권[*]

숙명여자대학교 화학과 [1]전북대학교 화학교육과

We have developed a simple and selective method for the electrochemical detection of hydrazine (HZ) using poly(dopamine) (pDA)-modified indium tin oxide (ITO) electrodes. Modification with pDA was easily achieved by submerging the ITO electrode in a DA solution for 30 min. The electrocatalytic oxidation of HZ on the pDA-modified ITO electrode was measured by cyclic voltammetry. In buffer solution, the concentration range for linear HZ detection was 100 μM–10 mM, and the detection limit was 1 μM. The proposed method was finally used to determine HZ in tap water to simulate the analysis of real samples. This method showed good recovery (94%–115%) and was not affected by the other species present in the tap water samples.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-215**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Determination of the Inorganic Arsenic with Solid Phase Extraction and LIBS

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목포대학교 화학과

The toxicity, bioactivity and mobility of arsenic are dependent on the chemical forms or species in which it exists. It is well known that the inorganic arsenic is more toxic than the organic arsenic. The ICP-MS coupled with chromatographic techniques has been used to perform the qualitative and quantitative determination of the arsenic species in various samples. However, it has been difficult to conduct a overall analysis due to matrix effects and took a long time to separate the arsenic species in various samples with the complex matrix. In this study, the solid phase extraction(SPE) membrane was used to separate inorganic arsenics, and those were detected by laser induced breakdown spectroscopy (LIBS). The samples were prepared using a buffer solution with phosphate buffer saline (pH 7.4) to separate arsenic species. The recovery efficiency of As(Ⅴ) by LIBS was 106.7 %. The separated As(Ⅲ) was identified by IC-ICP-MS. From the results, it was confirmed that inorganic arsenic species could be separated and detected using SPE membrane and LIBS.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-216**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and characterization of graphene-enfolded mesoporous TiO2 microsphere as anode material for Li secondary batteries

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계명대학교 화학과

In this study, graphene-bonded and enfolded mesoporous anatase TiO2 microsphere (GMTMs) composites have been synthesized without using any cross-linking reagent, by using graphene oxide (GO) and titanium glycolate microsphere (TGMs) as a precursor. Monodispersed and uniform mesoporous TiO2 microspheres with a tunable diameter were fabricated by the facile aqueous route, nano-particle microspheres are interconnected 10-20 nm in size. TGMs diameter tuned from 100 to 800 nm with consistent size and morphology by changing the amount of water. GO sheets were enfolded on TGMs by covalent bond after a subsequent refluxing. Crystallization of TiO2 and reduction of GOMTMs was dramatically marked up by hydrothermal and calcination in an Ar atmosphere. The physicochemical properties were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Field emission scanning electron microscopy (FE-SEM), Transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy. Surface areas were also measured by BET method. The electrochemical performance of TGMs composites as anode for Li secondary batteries were investigated by cyclic voltammetry, galvanostatic charge/discharge, and impedance spectroscopy. TGMs composite with higher surface area showed better electrochemical performance in charge capacity and cycle ability. AcknowledgementsThis research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (NO.2015035858)

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발표코드: **ANAL.P-217**
발표분야: 분석화학
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Setting up Overhauser Dynamic Nuclear Polarization Nuclear Magnetic Resonance Systems

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낮은 에너지를 사용하는 Nuclear Magnetic Resonance(NMR) 기법은 분자 구조와 운동을 비파괴적으로 관찰할 수 있으며, 비결정 시료 또한 분석이 가능하고, 관찰하고자하는 핵종을 선택 할 수 있어 선택성이 높다는 등의 장점을 가지고 있다. 하지만 NMR 은 낮은 에너지의 주파수를 사용하기 때문에 낮은 감도로 핵스핀 신호를 얻는다는 단점을 가지고 있다. 이러한 단점을 보완하기 위해서 본 연구에서는 전자스핀과 핵스핀의 상호작용을 통해 NMR 신호를 수십에서 수백 배까지 증폭시키는 장비인 Overhauser Dynamic Nuclear Polarization(ODNP) NMR 시스템을 Electron Paramagnetic Resonance(EPR) 장비에 NMR 부품(RF Pulse 모듈, NMR tuning box, ODNP NMR probe 등)을 결합하는 방법을 사용하여 ODNP NMR 을 구축하고자 한다. ODNP NMR 에서는 스핀표지자의 전자스핀 중심 반경 약 1 nm 내의 핵 스핀들과 주로 상호작용을 하여 NMR 신호가 증폭된다. 따라서 스핀표지자를 이용하여 측정하고자 하는 국소 부위를 지정할 수 있으며 고분자 물질내의 물의 확산속도, 용매 따른 단백질과 물의 결합 변화 등을 측정하는데 활용 할 수 있다.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-218**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Proton Nuclear Magnetic Resonance Spectroscopic Investigation of Inner Channel-Surface Change of Nafion upon Chemical Degradation

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고분자 전해질 막은 연료전지의 핵심 구성 소재로 많이 사용하는데 장시간의 연료전지 운영에 의하여 열화가 일어날 수 있다. 대표적인 고분자 전해질 막인 Nafion(나피온)의 경우, 수 많은 연구 결과에서 열화 산물로 나피온의 SO_3H 가 떨어지고 OH 로 대체되어 생긴 CF_2OH 를 주로 보여주었다. 하지만, 최근 문헌에서는 CF_2H 도 열적 열화의 산물임을 새롭게 제시하였다.이를 바탕으로 본 연구에서는 화학적 열화에서도 CF_2H 가 생성 되는지와 이 때, 친수성 채널 안에 있는 물이 받는 영향을 보고자 하였다. Fenton 반응을 1, 3, 6 시간 동안 진행하여 준비한 모든 나피온 시료에서 ~6.9ppm 에 CF_2H 의 신호가 나오는 것을 ^1H magic-angle spinning nuclear magnetic resonance spectroscopy 를 이용하여 확인하였다. 또한 Fenton 반응이 진행됨에 따라 나피온이 함유하는 물의 함량 (λ′)은 감소하여 Fenton 반응을 6 시간 시킨 시료의 경우, λ′이 0 으로까지 감소하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-219**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Investigation of Electrochemical Reactions in Direct 2-Propanol Fuel Cells(DPFCs) by ^{13}C Nuclear Magnetic Resonance Spectroscopy

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알코올 중 propanol 은 methanol, ethanol 에 비해 물과 이산화탄소만 생성하는 완전한 산화를 한다면 전자를 생산할 수 있는 에너지 발생 밀도가 크다는 이점을 가진다. 하지만 실제로는 propanol 연료전지의 경우 대부분 불완전 산화가 일어나고, 전극의 피독 현상이 일어나며, 연료가 양극에서 음극으로 넘어가는 크로스오버 현상이 일어나는 문제가 있다. 따라서 본 연구에서는 다양한 조건에서 2-propanol 연료전지를 운영하며 전기화학적 장비를 통해 얻은 정보와 양극과 음극 배출액의 ^{13}C Nuclear Magnetic Resonance (NMR) 스펙트럼들로부터 생성물의 규명 및 정량 분석을 수행하였다. 이를 통하여 연료극과 공기극 배출액의 화학적 조성이 연료전지의 성능에 따라 어떻게 변하는지 추적하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표분야: 분석화학
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SERS-based immunoassay for the simultaneous detection of two prostate-specific antigens in clinical serum

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Numerous studies showed that the clinical accuracy of the prostate-specific antigen (PSA) determination can be improved by measuring the ratio of either free PSA (f-PSA) or complex PSA (c-PSA) relation to total PSA (t-PSA). Enzyme-linked immunosorbent assay (ELISA) and photoluminescence bioassays have been widely used for the quantitative analysis of PSA in clinical laboratory. However, those techniques have some technical drawbacks such as poor signal-to-noise ratio, limit of detection and simultaneous multiplex detection capability. Thus, scientists and medical doctors are still concerned about the ways to improve the PSA immunoassay test for the precise diagnosis of prostate cancer. In this work, a novel SERS-based immunoassay platform, using gold nanoparticles and magnetic beads, has been developed for the simultaneous detection of f-PSA and c-PSA. Here, XRITC- and MGITC-labelled gold nanoparticles have been used as SERS nanotags for the dual PSA marker assay. On the other hand, magnetic beads have been used as supporting substrates for the high density loading of immunocomplexes. Using this simultaneous assay platform, the SERS-based assay data for 30 clinical samples were obtained and compared with those measured by the chemiluminescence instrument installed in clinical laboratory. Compare with a parallel assay, the simultaneous assay shows more precise result and also has better reproducibility. This SERS-based technique provides a new insight for the fast and accurate diagnosis of prostate cancer.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-221**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

SERS-based immunosensor for the highly sensitive detection of mycotoxin using three-dimensional nano-pillar array chips

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Mycotoxins such as ochratoxin A, aflatoxin B1, fumonisin and others are well-known dangerous food contaminants that usually occur in trace amounts from nanograms to micrograms per gram of food. Due to their teratogenic and carcinogenic properties, mycotoxins present a serious hazard to human and animal health. The conventional detection methods such as high-performance liquid chromatography, mass spectroscopy and ELISA are extensively used for their quantitative analysis but they are rather expensive or time consuming; therefore, a new detection technique is still needed for the rapid and sensitive detection of Mycotoxins. For this purpose, we designed a novel SERS-based immunosensor for mycotoxin detection by combining a three-dimensional (3D) nano-pillar array chip with a surface-enhanced Raman scattering (SERS) detection technique. Upon target mycotoxins and mycotoxins antibody introduction, a competitive-type immunoreaction was implemented between the target and the immobilized mycotoxins-BSA on the 3D nano-pillar array chip. After this reaction, secondary antibodies conjugated on SERS nanotags were captured on the 3D nano-pillar array chip surface, forming a confined 3D plasmonic field, leading to the enhanced electromagnetic field on the 3D pillar surface. This work is expected to be a potentially useful tool for the rapid and sensitive detection of various mycotoxins.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Various analytical methods for the determination of the arsenic species in rice

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목포대학교 화학과

The qualitative and quantitative determination of the total arsenic as well as the arsenic species in rice has been very important. However, it has been troublesome due to the matrix interference. In this study, the various analytical methods including the internal standard method and standard addition method have been investigated for the determination of arsenic species in rice. The four different arsenic species in rice have been separated by ion chromatograph, then detected by ICP-MS (inductively coupled plasma mass spectrometry). In addition, the various extraction methods by the nitric acid and the malonic acid have been also investigated. The quality control for rice was done with certified reference material (NIST 1568b CRM). The malonic acid extraction method showed 83 % recovery for the total arsenic, but only 58% recovery for inorganic arsenic. The nitric acid extraction method showed the overestimated results of 114 % recovery to total arsenic. We have used the nitric acid extraction method using arsenobetain as internal standard to improve the accuracy. Thus, we have acquired 96% and 66% recoveries for the total arsenic and inorganic arsenic, respectively. In addition, we have used the standard addition method to reduce the matrix interference. We have acquired 127 % and 111 % recoveries for the total arsenic and inorganic arsenic, respectively.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-223**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Amperometric antibiotics sensor using liquid/gel interfaces

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경북대학교 화학과

본 포스터에서는 서로 혼합되지 않는 두 전해질 (수용성 액체/유기성 젤) 계면에서 전하를 띈 항생제가 선택적으로 이동하는 반응에 따라 변화하는 전류값을 측정하는데 기반을 둔 이온 선택적 전류법 센서 개발에 관한 연구를 나타냈다. 수용성 액체와 유기성 젤 사이에 계면을 형성하고 수용액 액체의 pH 가 변할 때 항생제 이온의 전하도 달라진다. 이를 검출하기 위해 특정 pH 에서 전압을 걸어주게 되면 항생제 이온의 농도에 따라 계면에서 전이하는 정도의 차이에 따라 전류가 어떻게 변화하는 지를 순환전압전류법(cyclic voltammetry)과 시차 펄스 벗김 전위법(different pulse stripping voltammetry)으로 정량적으로 분석하였다.

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알칼라인 이온성 액체의 합성

김경민 이송하[1] 이혜진[1,*]

경북대학교 일반대학원/화학과 [1]경북대학교 화학과

본 연구실에서는 보다 쉬운 방법으로 여러 가지 성질(열에 잘 견디며, 낮은 증기압, 높은 이온전도도, 환경 친화적)을 지닌 점성질의 이온성 액체를 개발하고 있다. 이 이온성 액체는 실온 이온성 액체라고도 불리우며 유기합성, 촉매, 연료 전지 외에 여러 분야에서 다양하게 이용되고 있다. 유(무)기 양이온과 유(무)기 음이온을 여러가지 (극성, 무극성)용매를 이용하며, 합성물을 pH, 전기전도도와 정성 분석을 통하여 합성유무를 확인해 보았다.

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발표분야: 분석화학
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액체 / 액체 계면에서의 Tetracycline 전달 및 감지 응용의 Voltammetric 연구

LIU XIAOYUN 이혜진*

경북대학교 화학과

두 가지의 혼화되지 않는 전해질 용액 (ITIES) 사이의 분극화 된 계면을 통한 이온 전달 과정은 다양한 유형의 이온 선택성 감지 플랫폼을 만드는데 이용되어왔다. ITIES 를 통한 이온 전달 반응은 약물 분자의 친 유성을 이해하기위한 강력한 도구로 사용될 수 있다. 다양한 금속 이온, 음이온 및 전반의 전하를 띄는 약물 분자를 포함한 광범위한 이온 종의 연구가 액체 / 액체 계면를 통해 이루어졌다. ITIES 에서 다양한 약물 종의 전이 반응에 대한 많은 전기 화학적 연구 결과가 보고되었지만 항생제 또는 기타 질병 치료제의 정량 분석을위한 감지 플랫폼으로 ITIES 의 설계를 보여주는 보고서는 거의 없다 .

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-226**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

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

최진영 김용재 박영호[1] 이창섭*

계명대학교 화학과 [1]한국국제대학교 제약공학과

Graphene has been reported as an excellent lubricant additive for reducing adhesion and friction when coated on various surfaces as an atomically thin material with low surface energy. We have developed graphene oxide (GO) grafted with long alkyl chains to improve dispersion in oil-base lubricant as largely enhanced lipophilicity. Alkyl functionalized GO is synthesized by reacting NH2-GO with butylchloride, octylchloride in ethanol under reflux, then 1.0x10-3 wt% of alkyl functionalized GO are added into the base oil (PAG oil) and ultrasonicated for dispersion. Chemical and structural properties of the synthesized alkyl functionalized graphene are investigated by Fourier transform infrared (FT-IR), 13C solid-state nuclear magnetic resonance (13C NMR), X-ray diffraction (XRD), and scanning electron microscope (SEM). The tribological tests are performed with a tribometer and the test mode is ball-on-disk. The van der Waals interaction between the octyl chains grafted on GO and the alkyl chains of base oil provided long-term dispersion stability so that the octyl functionalized GO showed better dispersion than butyl functionalized GO. The octyl functionalized GO also decreased both friction and wear considerably under the rubbing contacts between ball and disk. Acknowledgements: This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2015035858).

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Synthesis and characteristics of reduced graphene oxide/mesoporous silica composites as anode materials for lithium secondary batteries

손빛나 현유라 배재영 박희구[1] 이창섭*

계명대학교 화학과 [1]계명대학교 화학시스템공학과

The reduced graphene oxide/mesoporous silica composites (rGO/m-S) as a high performance anode for lithium secondary batteries have been synthesized. The rGO/m-S composites with different mass ratios are dissolved in distilled water and coated on a Nickel foam via a simple dip-coating method. Nickel foam is used as a current collector and template for the electrode fabrication. The physicochemical characteristics of the rGO/m-S composites were analyzed by scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD), Raman spectroscopy, N_2-sorption and X-ray photoelectron spectroscopy (XPS). A three-electrode cell, as a half cell, was assembled by using rGO/m-S composites as the anode active materials of lithium secondary batteries in a glove box filled with Ar gas. The prepared rGO/m-S materials were used as the working electrode. Lithium was used as the counter and reference electrodes. A glass fiber separator was used as the separator membrane. 1 M $LiClO_4$ was used as the electrolyte and dissolved in a 1:1 volume mixture of ethylene carbonate:propylene carbonate 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. Li secondary batteries prepared with mixed rGO/m-S composite showed better electrochemical performance than the case of multilayered rGO/m-S composite. Acknowledgements This research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2015035858).

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발표코드: **ANAL.P-228**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Amperometric detection for antibiotic molecules using carbon modified electrode

Sabrina Hayati 이혜진*

경북대학교 화학과

An electrochemical biosensor was developed for detection of antibiotic molecules using sandwich assay format involving two bioreceptors for the target molecules. This sandwich format was examined on carbon screen printed carbon electrode (SPCE) surface. The binding of antibiotic molecule to both bioreceptors were analyzed by cyclic voltammetry and different pulse voltammetry with different target concentrations. Quantitative analysis of the target concentrations is also reported.

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Detection of antibiotic molecules using metallic nanoparticles modified screen printed carbon electrode

Yun Pei 이혜진*

경북대학교 화학과

Antibiotics are used to treat bacterial infection, while the abuse can cause a lot of side effects. An amperometric sensor fabricated on gold nanoparticle(NPs) modified screen printed carbon electrodes(SPCEs) is demonstrated for the detection of antibiotic molecules. The developed sensor’s electrochemical characteristics and performance were thoroughly investigated using cyclic voltammetry and differential pluse voltammetry.

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The synthesis of polydopamine to composite with multi-walled carbon nanotubes for modification of the glucose dehydrogenase into the electrode

이창준 전원용[1] 최영봉 김혁한[*]

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Polydopamine (PDA) was used as a biocompatible polymer that has been used in various fields ranging from material aspects, drug delivery, and bio-sensing. We has used as a biosensor multi-walled carbon nanotubes (MWCNTs) coated with PDA to improve sensitivity and reproducibility. MWCNTs was easily coated with PDA at room temperature by mildly stirring. The PDA immobilized MWCNTs (PDA/MWCNTs) solution was loaded onto indium-tin oxide (ITO) electrode. And after using mixed solution with 1-ethyl-3-(3-dimethyl aminopropyl) carbodiimide (EDC) and N-hydroxysuccinimide (NHS) to activate PDA/MWCNTs/ITO electrode, GDH was modified to the electrode. The morphological and thermal characterization of GDH-PDA/MWCNTs/ITO electrode was measured by field emission scanning electron microscope (FE-SEM) and thermogravimetric analyzer (TGA), respectively. And the electrical signal was checked by cyclic voltammetry (CV). Also, GDH-PDA/MWCNTs/ITO electrode wasn't affected by interferences such as ascorbic acid (AA) and uric acid (UA). Therefore, our study has shown that possibility for applying as a biosensor.

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Theinterface correlation between multi-walled carbon nanotubessize with hydrophilic polymer and dispersion

조호진 전원용[1] 최영봉 김혁한[*]

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Abstract: The hydrophilic dispersion of multi-walled carbon nanotubes (MWCNTs) have been studied causing its biocompatible properties for applying as biomaterials. In this study, the interface correlation between dispersion and multi-walled carbon nanotubes which has another size were investigated. The MWCNTs was treated by ultrasonic with hydrochloric acid (HCl) to control the size of that. The different size of MWCNTs were composited with poly(acrylamide)-poly(vinylpyridine) (PAA-PVP) hydrophilic polymer. The physicochemical characterization of PAA-PVP composites with MWCNTs were examined by particle size analyzer (PSA), X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM).And electrochemical impedance was measured by potentiostat. Finally, the zeta potential was used for interface correlation between MWCNTs size and dispersion. The results showed that the size of MWCNT for dispersion is very important.

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

황은정 김수연 김성훈[1] 박영호[2] 박희구[3] 이창섭[*]

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We have performed a study of a silica/carbon nanocoils (SiO_2-CNC) nanocomposite as a potentially high performance anode for rechargeable lithium secondary batteries. Carbon nanocoils were grown via chemical vapor deposition (CVD) method. Acetylene (C_2H_2) and Sulfur hexafluoride (SF_6) were flowed into the quartz reactor of a tubular furnace heated to 550 ℃ at 100 torr and maintained for 60 min to synthesize CNCs. CNCs were then put into the Tetraethyl orthosilicate (TEOS) to synthesize SiO_2-CNCs composite. The electrochemical characteristics of SiO_2-CNCs composites as an anode of Li secondary batteries were investigated using three-electrode cell. The SiO_2-CNCs composites loaded on Ni foam were directly employed as an working electrode without binder. As the counter and reference electrode used lithium foil. 1M $LiClO_4$ was employed as electrolyte and dissolved in a mixture of propylene carbonate (PC): ethylene carbonate (EC) in a 1:1 volume ratio. Glass fiber separator was used as the separator membrane. The galvanostatic charge–discharge cycling and cyclic voltammetry measurements were carried out at room temperature by using a battery tester. The morphologies, compositions and crystal quality of the prepared SiO_2-CNCs composites were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), energy X-ray diffraction (XRD), dispersive spectroscopy (EDS), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). As a result electrochemical performance of SiO_2-CNC was batter than existing carbon nanofibers and carbon nanocoils.AcknowledgementsThis research was financially supported by the Ministry of Education, Science Technology (MEST) and National Research Foundation of Korea (NRF) through the Human Resource Training Project for Regional Innovation (No. 2015035858)

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrochemical Studies on Anti-Cancer Drug Transfer Across Water/Oil Interface

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In this study, the ion transfer mechanism of an anthracycline derived anticancer drug at a polarized interface between two immiscible electrolyte solutions (ITIES) has been investigated. The voltammetric technique has been applied to study the ionization of the drug molecule at different pH of aqueous solution and organic solution interface. Some of preliminary results were demonstrated and a potential analytical purpose for sensing application of this work was also investigated in this work.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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A SERS-based magnetic immunoassay of fraction 1 antigen for Yersinia pestis utilizing integrated droplet microfluidics

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The combination of surface-enhanced Raman scattering (SERS)-based detection technique with lab-on-a-chip platform provides an ideal mechanism for achieving rapid, sensitive and reproducible assay 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, and its application to clinical diagnostics. 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 device was designed and fabricated for a sequential immunoassay processing in an automatic manner. This device is composed of six distinct compartments including droplets generation, mixing, merging, isolation, separation, and detection. Herein, we report a novel SERS-based droplet microfluidic device for fully automatic immunoassay in the microfluidic channel. For the proof-of-concept, the device was applied to the detection of the fraction 1 antigen of plague marker which is well known as an important anti-phagocytic antigen of Yersinia pestis.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-235**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

In-line coupled single drop microextraction and large volume sample stacking using an electroosmotic flow pump in capillary electrophoresis-mass spectrometry

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We introduce a method to obtain high sensitivity in capillary electrophoresis-mass spectrometry (CE-MS) by coupling of single drop microextraction (SDME) and large volume stacking using an electroosmotic flow pump (LVSEP) thereby sample cleanup and preconcentration before and after sample injection was achieved simultaneously. SDME was performed with a pentanol drop (as an organic solvent) at the tip of a fused silica capillary, which was immersed in the aqueous donor phase. A Teflon tubing sleeve was placed around the inlet capillary as a hydrophobic support. After SDME, large sample volume of enriched pentanol extract was injected hydrodynamically into the capillary and then further concentrated by LVSEP. In LVSEP, the adverse effects of a long sample matrix plug were overc ome by pumping the plug out of the separation capillary to the inlet vial using the electroosmotic flow under a potential of reverse polarity. Therefore, for the drop formation and the sample matrix removal, it was necessary to supply a backup run buffer from the outlet of the capillary, which was not trivial in most CE-MS system. We solved this difficulty simply by placing a vial supplying a backup run buffer during the drop formation and matrix removal processes without any physical modification of a conventional sheath liquid CE-MS interface. After the double sample preconcentration by SDME and LVSEP, several hundred–to thousand–fold enrichments were achieved for anionic analytes including chlorophenols.

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iCCM-based isotope dilution mass spectrometry for absolute quantification of human growth hormone and brain natriuretic peptide-32 in human plasma

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Isotope dilution mass spectrometry (ID-MS) has been used as a primary method for the absolute quantitative determination. Although the conventionally absolute quantification (e.g., synthetic proteins or peptides) or stable isotope labeling methods (e.g., ICAT, mTRAQ) in quantitative proteomics have been considered as a reliable approach in shotgun proteomics, these methods have unfortunately several bottlenecks such as imperfect labeling, and time consumption of labeling for proteome samples. To improve above-mentioned problems, we applied the carbamidomethylation-based isotope labeling (iCCM) for absolute quantification of hGH and BNP-32 in human plasma in this study. To evaluate the iCCM labeling for absolute quantification, plasma sample was first labeled with iodoacetamide (IAA) as carbamidomethylation (CM), while both human growth hormone (hGH) and brain natriuretic peptide-32 (BNP-32) standards were isotopically alkylated with IAA isotope (IAA-13C2D2) as iCCM, followed by spiking those iCCM-labeled standards to plasma sample labeled with CM. The resulting plasma sample was directly performed tryptic digestion and subsequently applied to nLC-ESI-MS/MS analysis so as to obtain the absolute amounts of both hGH and BNP-32. In conclusion, iCCM-based ID-MS provides the simple, rapid, and high reproductive method for the assessment of the ratio of CM/iCCM, resulting in absolute quantification of hGH and BNP-32.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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Efficient use of separation space in two-dimensional liquidchromatography system for extensive and efficient proteomicanalyses

이한겨레 이상원*

고려대학교 화학과

Proteomics aims to complete profiling of the protein content and their modifications in cells, tissues, and biofluids and to quantitatively determine changes in their abundances. This information reveals cellular processes and signaling pathways and serves to identify candidate protein biomarkers and/or therapeutic targets. Therefore, analysis should be comprehensive and efficient. Here, we present a novel online two-dimensional reverse-phase/reverse-phase liquid chromatography separation platform, employing a newly developed online non-contiguous fractionating and concatenating device (NCFC fractionator). In bottom-up proteomics analyses of a complex proteome, this system provided significantly improved exploitation of the separation space of the two RPs, resulting in a considerable increase in the numbers of peptides identified compared to a conventional contiguous 2D-RP/RPLC method. The fully automated online 2D-NCFC-RP/RPLC system bypassed a number of labor-intensive manual processes (offline fractionations, poling, clean-up, drying/reconstitution, and autosampler fraction injection) required with previously described offline 2D-NCFC-RP/RPLC method, offering minimal sample loss and highly reproducible 2D-RP/RPLC experiments.

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Development of advanced proteome-to-genome mapping technologies and application to proteogenomic characterization of early onset gastric cancer

문동기 이한겨레 이상원*

고려대학교 화학과

Next-generation sequencing and MS-based proteomics have been increasingly adopted as powerful technologies for characterizing cancer genome and proteome. Also there have been endeavors for integrating genomic and proteomic data to achieve comprehensive understandings of cancer. To this end, sensitive, extensive, and quantitative profiling of proteome are needed. In this study, advanced proteome-to-genome mapping (P2G) technologies were developed, including standardized proteome sample preparation procedure, serial enrichment of PTMs, highly sensitive LC-MS/MS analysis platform, and improved post-experimental peptide identification tool. Developed P2G mapping technologies were applied for characterizing proteome of early onset gastric cancer. Global proteome, phosphoproteome and N-glycoproteome profiling were performed for paired tumor and adjacent normal tissues of 80 patients. Obtained proteome profiles were integrated with genomics data (e.g. exome and mRNA data), which provided additional knowledges on cancer biology that were not obtainable by genomic data only.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-239**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Multiplex Quantitative PCR using Temperature Sensitive Primer/Probe-Supplying Hydrogel Particles for Pathogenic Infection Diagnosis

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한국과학기술연구원(KIST) 바이오마이크로시스템연구단 [1]한국과학기술연구원 바이오마이크로시스템연구단

For diagnostic objective and system biological research, it becomes very important to analyze diverse targets with limited amounts of sample in a single trial. Solid phase PCR (SP-PCR) has potential to increase the number of targets analyzed at the same time by using its solid characteristics, for example, array qPCR chip. Its use, however, has critical limitation of poor amplification efficiency, so it is not suitable for quantitative PCR (qPCR) analysis which is required to high PCR efficiency and precise resolution. Here we introduce new versatile qPCR method based on hydrogel particles act as individual reaction chambers. It has high multiplicity and great PCR efficiency though all the specific primers and probes are immobilized. At the PCR thermal condition, immobilized primers and probes are released from temperature sensitive materials for supplying primers and probes. PCR efficiency is over 92% and there are not undesirable byproducts thanks to ‘right primers supplying to right place only’ system. Several different targetting hydrogel particles can be used for multiplex analysis by being located in a single reaction channel.For applications, four typical malaria subtypes (P. f, P. v, P. m and P. o) were distinguished in a single reaction within 30 minutes. Since target-specific hydrolysis probes were used, it made our method better reliability and consistency even with clinical samples. We analyzed tens of samples originated from different malaria patients and normal people for a control and we successfully distinguished each patient’s subtypes. This technology will be widely used in SP-PCR area due to its excellent perfomances and convenient technical accessiblity.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Influence of sedimentation on the cellular association and endocytosis mechanisms of silver nanoparticles: Flow cytometry and ICP-MS study

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Recently, nanomaterials have attracted increasing interest and widely used in many applications, such as nanomedicine as well as consumer products. However, their accumulation in the environment raises concerns on the potential hazards of nanomaterials on biological and environmental systems.1 Silver nanoparticles (Ag NPs) are widely used as antimicrobial agents, laundry detergents, wall paint and clothing such as underwear and socks.2 Notwithstanding the increasing use of Ag NPs in consumer products and potential risk of human exposure, there is no quantitative understanding on their cellular association mechanism and resultant toxicity .3 To better understand these phenomena, it is prerequisite to develop measurement method and perform quantitative analysis of intracellular Ag NPs.4The purpose of this study is to investigate the influence of nanoparticle sedimentation on their cellular association and related endocytosis mechanism, when A549 cells were exposed to Ag NPs. We have measured the dispersion stability, hydrodynamic sizes, and surface charges of Ag NPs using UV-Vis spectroscopy, dynamic light scattering (DLS) and Zeta-potential. We also performed flow cytometry (FCM) and inductively coupled plasma – mass spectrometry (ICP-MS) measurements to quantify cellular Ag NPs under various exposure conditions. Inhibitor assays on endocytosis mechanisms were also conducted and confirmed with flow cytometry (FCM) and bio-transmission electron microscopy (bio-TEM), which provided us useful insight on the cellular uptake mechanisms of Ag NPs in A549 cells.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-241**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Physicochemical characterization of ZnO nanoparticles and their toxicity assessments using human lung epithelial cells(A549)

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Zinc oxide(ZnO) is one of the widely-used engineering nanoparticles(NPs), which is commonly used as ingredients of sunscreen or base make-up products to absorb UV radiation. In this study, Physicochemical characterization of ZnO nanoparticles (25, 50, and 150 nm) and their cellular association with human lung epithelial cells (A549) was investigated. For the ZnO nanoparticles with different surface charge and hydrodynamic size, single particle ICP-MS experiment was performed to obtain concentrations of ZnO particles and Zn2+ ion. MTT assay and flow cytometry (FCM) measurements were performed for A549 cells exposed to ZnO NPs for 24 hours. The measurement of side scattering (SSC) intensity in FCM is used as a method for the quantification of cellular ZnO NPs. Transmission electron microscope (TEM) was also used to observe the cellular association of ZnO particles. By using these integrated testing methods, we can provide better insights on the effect of ZnO NPs on biological systems.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

ISDD 모델링과 라만분광법을 이용한 탄소나노튜브의 effective dose 값 비교연구

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나노물질이 인체에 미치는 영향을 이해하기 위해서, 생체 외에서의 세포를 기반으로 한 실험이 행해지고 있다. 세포가 나노물질에 노출되었을 때, 이 나노물질이 세포에 직접적으로 전달되는 양을 'effective dose'라고 한다. 이 논문에서는 실용성이 뛰어난 물질로 알려진 탄소나노튜브(CNT)에 대하여 ISDD (in vitro sedimentation, diffusion and dosimetry) 모델링을 이용해서 구한 이론적인 effective dose 값과 라만분광법 실험을 이용해서 구한 실험적인 effective dose 값을 비교하여 ISDD 모델링의 실용성을 알아보고자 하였다. 우선 ISDD 모델링을 진행하기 위해서 고순도의 CNT 와 RPMI-full media 용매를 합친 샘플을 이용하였고, Effective dose 를 계산하기 위한 인자로 effective density 값을 얻기 위해서 VC(volumetric centrifugation) Method 을 사용하였다. Effective density 값등의 인자들을 ISDD 모델링의 식에 넣어주면 Effective dose 값에 해당하는 (number, surface area, mass) 값들을 구할 수 있다. 그리고 라만 분광법을 이용해서 침전된 CNT 의 양을 측정함으로서 effective dose 를 실험적으로 측정할 수 있으며, 결과적으로 구한 effective dose 측정값을 ISDD 모델링을 이용한 예측값과 비교를 함으로서 ISDD 모델링의 실용성이 있는 지 확인할 수 있었다.Reference: 1) Glen DeLoid et al, Nat. commun, 2014, 5, 35142) A.l. Lopez-Lorente et al, Analyst, 2014, 139, 290

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-243**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of Buckypaper using MWCNTs with Multivacancy Defects for Filtering Ultrafine Particulate Matter

송민우

수원대학교 신소재공학과

Our ultimate goal of this study is to fabricate buckypaper using multivacancy multi-walled carbon nanotubes (MWCNTs) for filtering ultrafine particulate matter application. First, MWCNTs-Co composites are fabricated by hydrothermal method and heat treatment in atmospheric conditions. Subsequently, cobalt oxide nanoparticles are removed by acid treatment. Through the processes, we can obtain multivacancy MWCNTs with high surface area. In addition, nitrogen-doped MWCNTs with multivacancy defects were obtained via chemical vapor deposition (CVD) method and the multivacancy MWCNTs were mixed with conducting polymer and ionic polymer. These surface modified and polymer composite MWCNTs with multivacancy defects are also employed to fabricate bukcypapes for filtering ultrafine particulate matter (PM 2.5). Here, we present the bukypapers using various multivacancy MWCNTs and filtration experimental data.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-244**
발표분야: 분석화학
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Flow cytometry study of the influence of agglomeration on effective in vitro dosimetry and cellular association of silver nanoparticles

HA KIEU MY 심유진 윤태현*

한양대학교 화학과

Nanoparticles (NPs) are becoming increasingly important in various biological and medical applications, from imaging and diagnostics to therapeutics and regenerative medicine, which requires comprehensive knowledge on how NPs interact with biological systems. In vitro assays are simple, fast and inexpensive approach to investigate these interactions and have been very useful in providing insights into the cellular interaction of NPs. However, they still face several challenges regarding their accuracy and reproducibility. One of the challenges is the effective dosimetry for inhomogeneously dispersed chemicals, such as NP dispersions. The actual NP concentrations that reach the adherent cells' surface are often different from the administered value, and one of the reasons for this discrepancy is the agglomeration and sedimentation of NPs. Exposure of NPs to cell culture media typically induce agglomeration and cause changes in their effective size and density. These parameters play important roles in their sedimentation and diffusion processes, which strongly influence their effective dose and cellular associations. Therefore, it is necessary to study how agglomeration of NPs affects their effective dose and cellular association, so that accurate and reproducible assay results can be generated.The objective of this study is to investigate the influence of Ag NP agglomeration on their effective in vitro dosimetry and their association with human lung cancer cells (A549). To address the influences of NP agglomeration on effective in vitro dosimetry, hydrodynamic size and effective density of Ag NP agglomerates in cell culture media were measured by dynamic light scattering (DLS) and volumetric centrifugation method (VCM) respectively, and were then used to estimate the effective in vitro dose of NP dispersions using a computational model developed by DeLoid et al. Moreover, to evaluate the impact of NP agglomeration on the sedimentation and diffusion processes, A549 cells were exposed to Ag NPs in upright and inverted configurations. Flow cytometry (FCM) side scattering (SSC) intensity measurement was used to quantify cellular association of Ag NPs. In the FCM technique, the SSC signal, which is related to the inner complexity of the cells, was combined with inductively coupled plasma mass spectrometry (ICPMS) technique and used to evaluate the association level of Ag NPs in A549 cells. On the basis of these FCM SSC and ICPMS measurements, we demonstrated the influence of agglomeration on the sedimentation and diffusion processes of NPs, and thus on effective in vitro dosimetry and cellular association of Ag NPs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-245**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

mPE-MMR to increase sensitivity and accuracy in peptide identifications from co-fragmented tandem mass spectra

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Mass spectrometry (MS)-based proteomics, which uses high-resolution hybrid mass spectrometers such as the quadrupole-orbitrap mass spectrometer, can yield tens of thousands of tandem mass (MS/MS) spectra of high resolution during a routine shotgun proteomics experiment. Despite being a fundamental step in MS-based proteomics, the accurate determination and assignment of precursor monoisotopic masses to the MS/MS spectra remains difficult. The difficulties stem from imperfect isotopic envelopes of precursor ions, inaccurate charge states for precursor ions, and co-fragmentation of MS/MS spectra. Here, we describe a composite method of utilizing MS data to efficiently assign accurate monoisotopic masses to MS/MS spectra, including those subject to co-fragmentation and unassigned charge state. The method, “multiplexed post-experiment monoisotopic mass refinement” (mPE-MMR), consists of the following: multiplexing of precursor masses to assign multiple monoisotopic masses of co-fragmented peptides to the corresponding multiplexed MS/MS spectra, multiplexing of charge states to assign correct charges to the precursor ions of MS/MS spectra with no charge information, and mass correction for inaccurate monoisotopic peak picking. When combined with MS-GF+, a database search algorithm based on fragment mass difference, mPE-MMR effectively increases both sensitivity and accuracy in PSMs and peptide identification from complex high-throughput proteomics data compared to conventional methods.

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장소: 일산 KINTEX
발표코드: **ANAL.P-246**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Novel tridoped TiO_2 nanoparticles with Er^{3+}-Yb^{3+}-Ce^{3+} for photodegradation of Rhodamine B

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창원대학교 화학과

Titanium dioxide (TiO_2) has been extensively used on photocatalyst applications, because it has relatively high photocatalytic actively, robust chemical stability, unexpensive and nontoxicity. However, TiO_2 has an energy band gap of about 3.2 eV due to the reason it mainly absorbs the ultraviolet portion of the solar spectrum and only a small amount of visible light. Thus, increasing photocatalytic efficiency by increasing light absorption ability of TiO_2 is necessary. In this study, Ce^{3+}, Er^{3+} and Yb^{3+} ions were doped simultaneously to TiO_2 for expanding light absorption range of TiO_2. The effects of synthetic temperatures, concentration of dopants in synthesis process of TiO_2 nanoparticles on photocatalytic efficiency for Rhodamine B were investigated. In addition, pH value of photodegradation medium was also optimized.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-247**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Relationship between in vitro and in vivo toxicity of carbon nanotube: a meta-analysis from literature data

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As the number of nano-products has been sharply increasing in recent years, there are more and more public concerns about the safety of nanomaterial and related products. Generally, toxicity of nanoparticles is evaluated through in vitro (experiments with cultured cells) and in vivo (experiments with living organisms) protocols which require much time and labor cost. With the development of in silico approach (building and applying computational models for the toxicity prediction of nanomaterials), time and labor cost for the hazard assessment could be reduced [1]. The relationship between in vitro and in vivo toxicity has not been clear yet. Carbon nanotube materials have been used widely in industry and household and become a good object of studying that relationship. Gernand et al [4] already did meta-analysis on in vivo toxicity of multi-wall carbon nanotube and made a prediction model based on random forest algorithm. In this study, we used Gernand data as main source of in vivo toxicity data of carbon nanotube and collected in vitro toxicity data from other literatures and did meta-analysis to find out relationships between in vitro and in vivo toxicity of carbon nanotube materials. This study will support for later research of correlating in vivo and in vitro toxicity of nanomaterials.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-248**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Highly selective determination of catecholamines using dithiol modified upconversion nanoparticles with metal ions

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창원대학교 화학과

Catecholamines are a well-known neurotransmitter and related mammalian central nervous system. Therefore, when the amount of catecholamines in tissues are abnormal, it is possible to cause several diseases including Parkinson’s diseases, chronic inflammatory diseases. However, catecholamine-secreting cells are converted tyrosine to L-DOPA and then to dopamine. Furthermore, epinephrine and norepinephrine are released by dopamine. Dopamine, epinephrine, and norepinephrine show different action in the nervous system, although all catecholamines are conducted both as hormone and neurotransmitter. Therefore, separation of catecholamines is required with highly sensitivity, simple, and fast analytical method. Upconversion nanoparticles (UCNPs), that convert near-infrared radiation (NIR) to visible, have been used the biological field. Furthermore, NIR irradiation has deeper penetration properties and less harmful to biological samples compared to UV excitation. Therefore, our goal is a determination for catecholamine respectively with various metal ions by upconversion luminescence (UCL). First, we developed a facile synthesis of Yb^{3+}/Er^{3+}-doped $NaLuGdF_4$ (UCNPs) coated with 1,2-ethanedithiol (EDT) to detection of catecholamines. Second, metal ions decorated UCNPs are conducted to the separation of dopamine and epinephrine from catecholamines.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-249**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Copper Coordinated Cationic Polyvinylpyrrolidone as a Novel Fluorescent Probe for Hydrogen Sulfide in Aqueous Solution

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창원대학교 화학과

A cationic polyvinylpyrrolidone (Cat-PVP) was prepared via Claisen- Schmidt condensation in super basic media and characterized using different spectra analyses (IR and ^{1}H-NMR). The prepared Cat-PVP was utilized to prepare a stable fluorescence copper coordinated cationic polyvinylpyrrolidone in aqueous media. The Cu-CatPVP was successfully utilized to detect hydrogen sulfide (H_2S) based on strong affinity between sulfur and copper. The quenching effect on the fluorescence intensity of the Cu-CatPVP probe showed very good linearity with H_2S concentrations in the range of 1−40μM, with detection limit as low as 0.13 μM. The presented probe promising selectivity toward H_2S over anions, biothiols as well as other amino acids in neutral media and was successfully applied for detecting the H_2S in real samples.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-250**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Upconversion Nanoparticles Functionalized with Novel Amphiphilic Polymers for Enhanced Biocompatibility and Bioimaging of KB Cells

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창원대학교 화학과

We have synthesized amphiphilic alginate (Al-NH-PEG-NH_2 and Al-NH-PEG-NH-FA)as the novel ligands to functionalize upconversion luminescent surface. Upconversion nanoparticles ($NaLuGdF_4$: Yb,Er,Cr) were capped with a thin polymer shell by replacing the oleate ligand of hydrophobic UCNPs by multidentate carboxylates of amphiphilic alginate polymers. Using amphiphilic alginate polymers as the surface ligands not just enhances the stability and biocompatibility of the UCNPs under physiological conditions but also displayed enhanced upconversion luminescent intensity. It was found that a maximum upconversion luminescence enhancement of 20-fold was obtained in comparison with the hydrophobic UCNPs. In order to demonstrate the targeted bioimaging capability of the functionalized-UCNPs, two cell lines (KB and HeLa) were employed for the investigations on the basis of their different folate receptor expression level. The results illustrated that the UCNP-Al-NH-PEG-NH-FA was specific in targeting KB cell lines more than HeLa cell lines under an excitation wavelength of 980 nm. The cell viability of two types of cells incubated with high concentration (300 $\mu g \cdot mL^{-1}$) of functionalized-UCNPs still remained above 85% after 24 h. The formation of stable water-dispersible UCNPs with enhanced emission, together with their amphiphilic and biocompatible polymer coating, is promising for building multifunctional nanostructures for cell imaging, therapy, and drug delivery.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-251**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Ultrasensitive fluorescence detection of heparin using CdTe quantum dots coated with amphiphilic polythiophenes

심지민 **Salah Mahmoud Tawfik Ahmed** 이용일*

창원대학교 화학과

A new strategy for the detection of heparin is developed by utilizing quantum dots (QDs) coated with amphiphilic polythiophenes. The amphiphilic polythiophenes (PTPQ2000)-coated CdTe QDs were synthesized by in situ polymerization of modified thiophene on the surface of CdTe QDs. The PTPQ2000-coated CdTe QDs has a tremendously enhanced fluorescence and improved biocompatibility compared to the uncoated CdTe QDs. The PTPQ2000-coated CdTe QDs was successfully utilized to detect heparin. The emission of PTPQ2000-coated CdTe QDs is found to be quenched upon addition of the polyanionic heparin, due to electron transfer via electrostatic and/or hydrogen bonding interactions between heparin and PTPQ2000-coated CdTe QDs. The fluorescence intensity quenched with the increase of heparin and a good linear relationship was observed for heparin detection in buffer solution and the limit of detection (LOD) is 0.75 nM. The selectivity results of the fluorescence assay revealed that our system displayed excellent fluorescence selectivity towards heparin over its analogues. This fluorescence "switch of" assay for heparin is label-free, less toxic, sensitive and selective, which can be used to detect heparin in biological systems.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-252**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Phospholipase A2-responsive UCNPs-loaded Phosphate Micelles for Prostate Cancer Cells Imaging

SHARIPOV MIRKOMIL Salah Mahmoud Tawfik Ahmed GerelkhuuZayakhuu 이용일*

창원대학교 화학과

Rare-earth upconversion nanoparticles (UCNPs) have been proposed as biological luminescent labels for the bioimaging application. However, their toxicity, low dispersion, and low selectivity call into question their suitableness in nanomedicine. Herein, UCNPs-loaded phosphate micelles formed from the secreted phospholipase A2 (sPLA-2) enzyme cleavable phosphate micelles to deliver UCNPs directly to prostate cancer cells has been reported. These phosphate micelles were designed from biocompatible materials. Through a dye micellization method, the CMC value of micelles was determined to be 6.38×10^{-4}M. The activity of (sPLA-2) enzyme toward the synthesized micelle was investigated and confirmed using LC-MS. TEM results showed that micelles have a size ranged between 50 to 80 nm; whereas UCNPs loaded micelles have from 60 to 100 nm. Bio-imaging experiments conducted on KB, HeLa, and 22Rv1 cell lines confirmed the selectivity of UCNPs-loaded micelles toward 22Rv1 cell line. Moreover, the non-selective binding of UCNPs towards cells with low expression of PLA-2 was significantly reduced and MTT assay results confirmed the biocompatibility of micelles.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-253**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Identification of C_{18} Ceramide with Metal Ions using Electrospray Ionization Mass Spectrometry

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창원대학교 화학과

Herein, electrospray ionization – mass spectrometry [ESI-MS/MS] is applied for the investigation of C_{18} – ceramide complexes with transition metal ions such as Mn^{2+}, Cu^{2+}, Co^{2+} and Ni^{2+}. The formation and fragmentation of doubly charged cluster ions of C_{18} – ceramide with metal ions will be studied by ESI-MS/MS in the positive mode. Tube lens offset voltage and concentrations of C_{18} – ceramide and metals are optimized to determine the best conditions for charged ions. The fragmentation pathways of metal ion complexes with C_{18} – ceramide and the compositions of these complexes are determined by collision induced dissociation (CID). All metal ions show the similar complexation with C_{18} ceramide. Consequently, MS/MS combined with ESI can be the most powerful technique to scrutinize transition metal ion complexes with C_{18} – ceramide. Experiments on metal cations have mostly been restricted to singly charged ions due to the significant experimental challenges in interpreting the structure and chemistry of multiply charged metal complexes, strongly suggests the need for studies using ESI-MS/MS.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-254**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Facile synthesis of $NaYF_4$:Yb^{3+}/Tm^{3+} upconversion nanoparticles coated with polyepinephrine for optosensing of Fe^{3+} ion

GerelkhuuZayakhuu 정다솜 정종원 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+}/Tm^{3+} doped $NaYF_4$ UCNPs coated with polyacrylic acid (PAA) was accomplished by the one-step hydrothermal method. Then polyepinephrine (PEP) formed on the UCNPs via self-polymerization of epinephrine. After polymer coated UCNPs showed enhancement of upconversion luminescence (UCL), and optimize condition was found. The successful synthesis of $NaYF_4$:Yb^{3+}/Tm^{3+}@PEP was used for optosensing of the Fe^{3+} ion. In detail, luminescence properties and morphology were discussed. From the obtained results, could be concluded that $NaYF_4$:Yb^{3+}/Tm^{3+}@PEP was successfully synthesized by the one-step hydrothermal approach, which is detected Fe^{3+} ion in aqueous system with high selective, sensitive, and simple. Furthermore, the $NaYF_4$:Yb^{3+}/Tm^{3+}@PEP showed relatively high cell viability. The high-quality of the synthesized UCNPs have prominent potential applications for optical nanodevices, bioimaging, and bioanalytic sensing.

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장소: 일산 KINTEX
발표코드: **ANAL.P-255**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

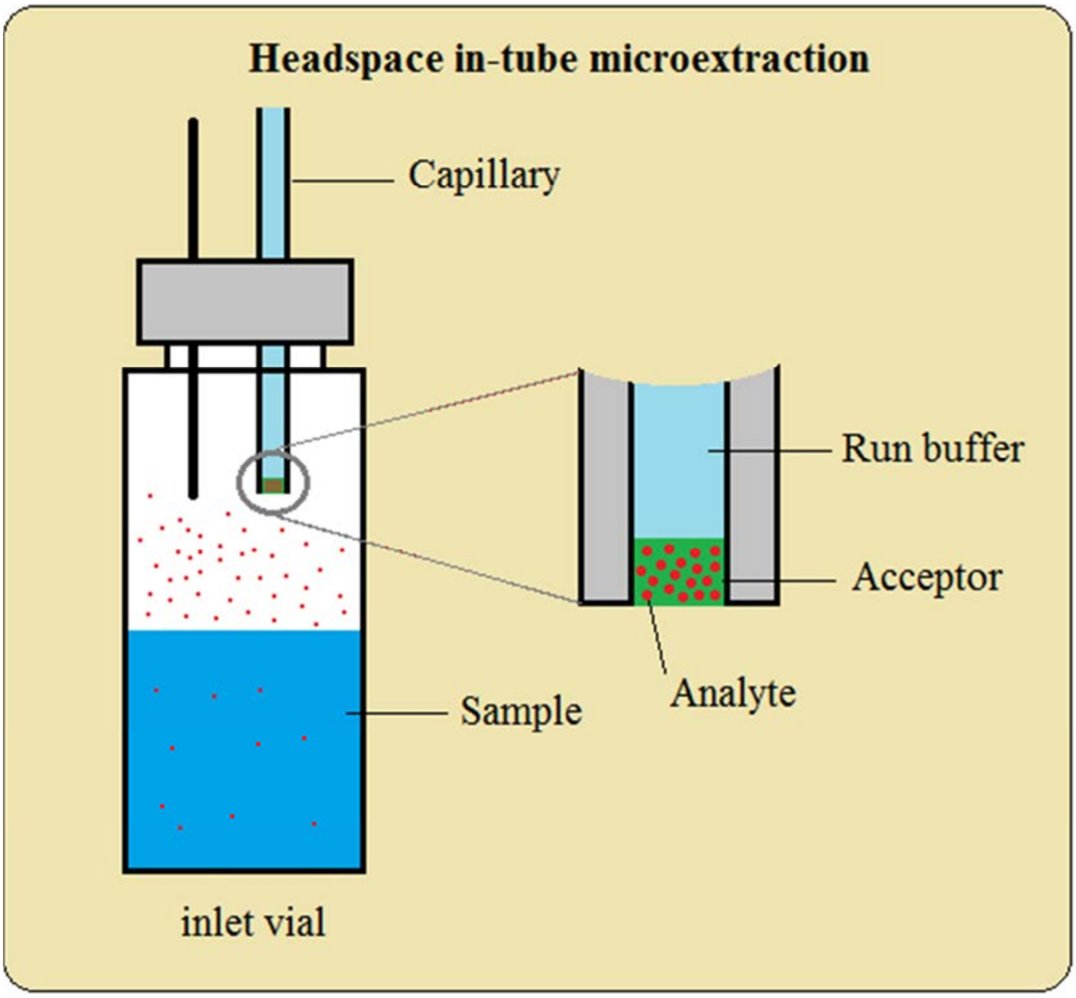
Determination of trichlorophenols in water samples using headspace in-tube microextraction followed by capillary electrophoresis

karimi maryam 정두수*

서울대학교 화학부

Chlorophenols are used widely in industry as intermediates in the production of dyes, plastics and pharmaceuticals, and are commonly found in pulp and paper mill wastewater, which pollute the groundwater sources. The harmonization of the analysis of chlorophenols in water is of importance due to the toxicity of these components and the presence in the aquatic environment. In the previous research, we demonstrated a fast simple preconcentration and microextraction method, head space in-tube microextraction (HS-ITME), which was initially used for determination of chlorophenols (CPs) and BTEX (benzene, toluene, ethylbenzene, and m-xylene) in wine and water samples, respectively. Rapidity, high enrichment factor, simplicity of operation and low cost are some of the advantages of this method. In this study HS-ITME is applied to determine six trichlrophenols in a water sample. At first, an acceptor phase was injected into the capillary in a desired duration of time. The capillary inlet is placed in the headspace above an acidified donor solution; volatile acidic analytes were extracted into the acceptor phase (a basic solution) in the capillary. After extraction, the analytes enriched in the basic acceptor plug were analyzed with capillary zone electrophoresis.

Some effective parameters on extraction, such as donor volume, donor pH, type of acceptor and its volume, waiting time, pre-injection volume, salt addition, extraction time and temperature were investigated. Also, the influence of adding organic additives on the headspace analysis of trichlorophenols is investigated.


Headspace in-tube microextraction
Capillary
Run buffer
Acceptor
Analyte
Sample
inlet vial

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장소: 일산 KINTEX
발표코드: **ANAL.P-256**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

MATLAB-based Statistical Analysis Software for Edible Oils Classification

손민희 오한빈*

서강대학교 화학과

Edible oils contain a variety of lipids, particularly diacylglycerols (DAGs) and triacylglycerols (TAGs). Different edible oils have their own signature lipid distribution. In this study, we acquired MALDI-TOF (Tinkerbell, Asta, Korea) mass spectra of 9 species of edible oils, such as sesame, perilla, olive, canola, grape-seed, sunflower-seed, corn, soybean, coconut oils. For the classification of edible oils using statistical analysis, we used principle component analysis (PCA), partial least square-determinant analysis (PLS-DA) and support vector machine (SVM). Using these statistical methods, statistical models were established. Based on those statistical analysis results, an edible oil analysis software was constructed using MATLAB. This software can not only visualize the acquired MALDI mass spectrum, but also readily classify unknown edile oils based on the PCA/PLS-DA/SVM statistical models by projecting the acquired spectrum components onto the established statistical models for the classification of edile oils.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ANAL.P-257**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

MALDI-TOF/TOF applications of TEMPO-assisted free radical initiated peptide sequencing (FRIPS) mass spectrometry

송인수 차상원[1] 오한빈*

서강대학교 화학과 [1]한국외국어대학교 화학과

Unlike CID-based peptide sequencing, TEMPO-assisted FRIPS makes use of a radical species for peptide sequencing. In this method, a peptide is conjugated with o-TEMPO-Bz-C(O)-NHS and thus generating o-TEMPO-Bz-C(O)-peptides. When o-TEMPO-Bz-C(O)-peptides is subjected to collisional activation, o-TEMPO-Bz-C(O)-peptides undergoes homolytic cleavage, forming ·Bz-C(O)-peptide. Then·Bz-C(O)-peptide produces a, c, x, and z-type products upon the secondary collisional activation. So far, ESI has been used for the TEMPO-assisted FRIPS MS. In this study, MALDI-TOF/TOF was performed on o-TEMPO-Bz-C(O)-peptides. It was revealed that MALDI ionization for o-TEMPO-Bz-C(O)-peptides was greatly affected by the matrix. 3-HPA(3-Hydroxypicolinic acid) was found to be a good matrix, whereas DHB, CHCA, showed a very low ionization efficiency. MALDI MS/MS of the detected o-TEMPO-Bz-C(O)-peptides yielded a, c, x and z-type products.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ANAL.P-258**

발표분야: 분석화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of a Dissolved Organic Matters (DOMs) Analysis Program Using a MATLAB Language

장인애 오한빈*

서강대학교 화학과

Dissolved organic matters (DOMs) is a complex mixture of degradation products from plants and animals and it plays a key role in the global carbon cycle. The ultra-high resolution mass spectrometer, such as Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS), is required to analyze DOMs in a river or ocean. Because the number of DOMs that exist in the mass spectrum is at least over 2000 peaks, an automatic analysis software is needed for the analysis of the numerous peaks of DOMs. Thus, we developed a software for the analysis of DOMs using a MATLAB language. In this study, we collected water samples of the Han River at Amsa located in the main stem and Jungnang located in the tributary. The collected water samples divided into two microtubes, and then one was treated C18 solid phase extraction (SPE) and the other was subjected to C18 SPE after microbal incubation for 5 days. Mass spectra were obtained by 15 T FT-ICR MS (SolariX XR, Bruker Daltonics, Germany) and various Van Krevelen diagrams were plotted using a home-coded MATLAB program. To conclude, the Han River of Amsa and Jungnang water samples were analyzed by a semi-automatic home-coded program, and a graphic user interface (GUI) will be added in the near future.

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Make Your Own Nano-LC MALDI Spotter Robot using a 3D Printer

이재웅 오한빈*

서강대학교 화학과

The 3D printing technology is growing very rapidly, and is bringing about significant advances in many research areas. On the 3d printing related website, the stories of making 3d printed parts and custom equipment have been posted. In this research, we made a DIY nano-LC MALDI spotter robot using 3D printed custom parts. Using this equipment, nano-LC and MALDI matrix loading can be conveniently coupled online and thus the separated eluents from nano-LC can be loaded automatically onto the MALDI plate. This DIY robot was made of only 3d printed parts and the parts on the online marketplace, so that anyone can make it and carry out maintenance easily and inexpensively. In this DIY robot, the loading speed can be readily controlled using a home-coded software. In addition, a camera is equipped so that the loading process can be monitored.

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Improved Performance of Dye-sensitized Solar Cell in Counter Electrode Using Upconverting Capability in Ln-FTO and FTO-UCNP Hybrid Nanostructures

NGUYEN THI THU THUY B.T.Huy 이용일*

창원대학교 화학과

Upconverting capability of hybrid nanostructure is promising potential candidate to dye-sensitized solar cell because of their unique properties to enhance of near-infrared light harvesting. In this paper, we reported a novel Ln-FTO and FTO-UCNP hybrid nanostructures and investigated their excellent optical and catalytic capability for using as the counter electrode in dye-sensitized solar cell (DSSC). FTO based on F-doped SnO_2 was used as special catalyst with excellent chemical stability, and high efficiency for counter electrode materials in dye-sensitized solar cell. These observations by IPCE and SPS demonstrated high effect Near-infrared light to electricity to upconversion counter electrode, even than Pt electrode in terms of low cost, simple preparation and high solar-to-electric power conversion efficiency (PCE). We proved that this novel upconversion hybrid nanostructure opened new era to excellent materials in dye-sensitized solar cell with upconvertiong capability, decent catalytic properties, and good conductivity.

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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

라만분광법을 이용한 의약품 제조 중 공정시료의 주성분 함량분석법 개발

임영일 한장희 박치서 김재진*

(주)종근당 품질관리팀

의약품 제조공정 중 주성분 및 부형제의 함량이 단위공정 중 변화되지 않고 일정하게 유지되고 있음을 확인하는 함량 및 함량균일성 시험은 중요한 품질관리의 항목이라고 할 수 있다. 이와 같이 공정 중 함량의 변화를 확인하기 위해 각 나라의 약전 및 우리나라의 대한약전에도 액체크로마토그래피(HPLC)를 이용하여 주성분의 함량을 시험하는 것을 의무화 하고 있다. 하지만 HPLC 방법은 목적물질을 기타물질과 완벽하게 분리해야 하는 실험조건을 찾아야 하고 목적물질이 컬럼을 통해 최적으로 분리되어 나타나는 머무름 시간 동안 시간이 소요되는 단점을 가지고 있다. 또한 이동상 용매의 조제 및 시료를 파괴해서 전처리하는 시간이 소요되고 기타 기기조건과 작업장 환경을 항상 일정하게 유지해야 한다. 이와 같이 분석시간이 많이 소요되고 기기 및 환경에 의한 분석 정확도에 영향을 줄 수 있는 HPLC 법을 부분적으로 대체하기 위해 분광학적 분석방법인 라만분광법을 이용하여 공정 시료의 주성분 함량분석 시험법 개발에 관한 연구가 진행되어지고 있다. 본 연구에서는 심혈관계 질환의 위험성을 감소시키는 atorvastatin 을 주성분으로 하는 제품의 제조공정 중 최종혼합 공정시료의 주성분 함량분석 연구를 진행하였다. 라만분광법의 단점인 형광을 나타내는 원료인 Microcrystalline cellulose(MCC)가 부형제로 포함되어 정량분석에 미치는 영향을 확인하였고, 확산반사 광역조사라만과 투과라만분광기로 측정 및 스펙트럼을 비교하였다. 표준샘플을 이용하여 정량모델을 수립하였고 모델의 정확성을 확인하기 위해 external validation 표준샘플과 습식과립, 건조, 혼합공정 후 샘플링 한 공정시료의 주성분 함량을 예측하여 정량모델의 정확성을 검증하였다.

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장소: 일산 KINTEX
발표코드: **ANAL.P-262**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Uranium age-dating of UO2 materials by determining Th-230/U-234 ratios using MC-ICP-MS

임상호[*] 한선호[1] 박진규 이치규

한국원자력연구원 원자력화학연구부 [1]한국원자력연구원 분석화학실

Various analytical methods for estimating production date of uranium materials for nuclear forensics purpose have been developed. These methods are based on the estimating of a daughter-mother radionuclide pair such as Th-230/U-234, Pa-231/U-235, Bi-214/U-234 and so on. Th-230/U-234 is often used isotope pair due to relatively rapid ingrowth of Th-230 and availability of traceer and spike. For derrmining highly accurate and precise Th-230/U-234 ratio, Th-230 has to be separated to remove interfering species from uranium samples. For this purpose, we adopted relatively simple and effective chemical separation method based on TEVA resin and optimized it.In this study, the optimized analytical procedure will be described including both chemical procedures and mass spectrometry analyses for Th-230/U-234 ratio of uranium oxide samples. In chemical procedures, pretreatment of uranium oxide sample, elution curve and recovery yield from optimized chemical separation and IDMS technique are discusssed. In mass spectrometry analysis, detailed uranium and thorium isotopic analyses with MC-ICP-MS (Neptune Plus, Thermo Scientific, Germany), calculation, data analysis are presented.

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발표분야: 분석화학
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Glycan Heterogeneity Differentiation Using Lectin-based SDC Separation and Glycopeptide level SDC Separation

정미선 조원련*

원광대학교 바이오나노화학부

Previous work in this group showed displacement phenomena in lectin affinity chromatography in glycoprotein level using LEL Lectin-based SDC Separation. However, the SDC can fail to differentiate between glycoforms of proteins with multiple glycosylation sites when a high affinity glycan is conjugated to a protein at one site and a low affinity glycan at another site in the same protein. The high affinity glycan will dominate binding of the protein to the lectin column and the low affinity glycan will be unrecognized. This problem can be solved with the digestion of the glycoproteins using self-packed trypsin column and glycopeptide Lectin-based SDC Separation. Human pooled plasma were digested with the self-packed trypsin columns without chemicals.

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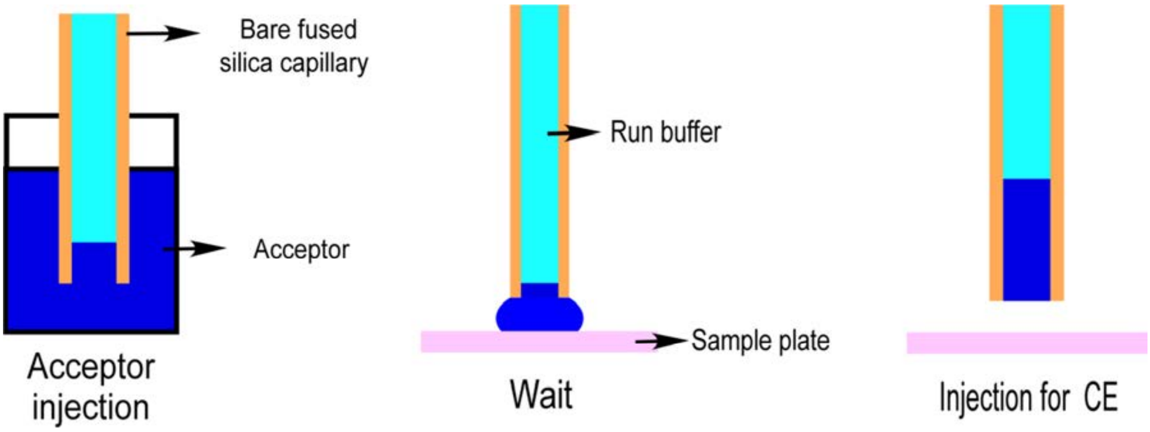
Liquid extraction surface analysis coupled with commercial capillary electrophoresis for direct analysis of solid surface samples rapidly

정선경 정두수[1,*]

서울대학교 화학부 [1]서울대학교 화학부

Capillary electrophoresis (CE) is well suited for the analysis of analytes in aqueous solutions. It is not easy to analyze a solid sample with CE since labor-intensive sample pretreatment processes are required. For example, a solid sample should be grounded, homogenized, centrifuged, extracted into an organic solvent, and then reconstituted into an aqueous solution suitable for CE. So we used liquid extraction surface analysis (LESA) that extracts chemicals on the surface of various solid samples without any sample pretreatment. Dried analytes doped on a surface were directly extracted to a hanging drop of extractant at the inlet tip of a capillary. After extraction, a small volume of acceptor was injected into the capillary and analyzed by a commercial CE instrument. LESA-CE was used to determine three species of insecticides, chlorantraniliprole, kresoxim-methyl, and pyraclostrobin. The U.S. Environmental Protection Agency (EPA) limits the allowable amounts of the insecticides to 4.0 ppm, 0.5 ppm, and 2.5 ppm respectively. For these water-insoluble analytes, micellar capillary electrophoresis (MEKC) was used and an on-line stacking method, analyte focusing by micelle collapse (AFMC) was combined to enhance the sensitivity. These three pesticides doped on sample plate were extracted with the inlet of a capillary and analyze directly with CE. Several parameters such as the condition of AFMC-MEKC, composition of acceptor, extraction time were optimized. The limits of detection (LODs) with LESA-AFMC-MEKC were 72, 23, and 29 ppb, respectively. Thus LESA-CE is a simple, sensitive and more rapid method for the analytes solid surface analytes without any pretreatment processes required for conventional analysis methods. The developed LESA-CE of high spatial resolution and immediate quantification ability is promising for the analysis of biological surfaces of cells and tissue, or even technical surfaces.


Bare fused silica capillary
Acceptor
Acceptor injection
Run buffer
Sample plate
Wait
Injection for CE

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장소: 일산 KINTEX
발표코드: **ANAL.P-265**
발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Real-Time Kinetic and Mechanistic Study of Decarboxylation Reaction of Pyruvic Acid using Hyperpolarization Technique

서형림 황수민 이영복*

한양대학교 바이오나노공학과, 응용화학과

Kinetic and mechanistic study of fast chemical or biochemical reactions is one of the major applications of NMR spectroscopy. In order to characterize the reactions, low-temperature NMR technique is traditionally utilized. However, the low-temperature technique is very limited to specific reactions due to solvent and solubility issues. Here, we demonstrate room-temperature kinetic and mechanistic study of decarboxylation reaction of pyruvic acid using dynamic nuclear polarization (DNP) technique. Hyperpolarization of pyruvic acid provides a sufficient signal-to-noise ratio for real-time detection of 13C NMR signals as the reaction progresses. This capability enables DNP method to be an attractive method for both kinetic and mechanistic study of various chemical or biochemical reactions.

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Silicon Nanoparticle based Magnetic Resonance Imaging Probe for Early-Stage Cancer Diagnosis

최익장 김도경 이영복*

한양대학교 바이오나노공학과, 응용화학과

Silicon-based nanoparticle has been attracting lots of interest in the field of magnetic resonance (MR) applications because of its specific features of biocompatibility and flexible surface chemistry. Since a core region of the crystalline Si NPs is mostly protected from paramagnetic centers on its surface defect sites, the Si NPs conventionally represent extremely long depolarization times, resulting in high MR signal-to-noise ratio with minimum background signals. In order to synthesize size-controlled Si NPs, we utilized magnesiothermic reduction of silica nanoparticles at various reduction temperature and time. In addition to the traditional synthetic approach, we produce 29-silicon enriched NPs with synthesized 29Si-TEOS for the purpose of additional signal enhancements. The enriched Si NPs in combination with hyperpolarization technique provide sufficient MR signals for *in vitro* and *in vivo* MR applications.

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장소: 일산 KINTEX
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발표분야: 분석화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Characterization of heterogeneous oligomerization of amyloid-β 1-40 and 1-42 using electrospray ionization mass spectrometry

허채은 김준곤*

고려대학교 화학과

Amyloid fibrillation of amyloid-β (Aβ) peptides has been accepted as the main cause of Alzheimer's disease (AD). Aβ40 is the most abundant form in Aβ peptides, while Aβ42 is highly relevant to the progress of AD. The ratio of Aβ40:Aβ42 in human brain is approximately 9:1, but the ratio of Aβ42 is increased in the brains of patients with AD. Since Aβ42 is more aggregation-prone than Aβ40, amyloid fibrillation of Aβ peptides can be promoted when increasing the ratio of Ab42. Additionally, it has been reported that the high ratio of Aβ40 inhibits the aggregation of Aβ42. However, the molecular interaction between Aβ40 and Aβ42 during the inhibition of Aβ42 fibrillation is still unclear. In this research, we demonstrate the role of Aβ40 during the fibrillation process of Aβ42. We monitored the fibrillation process of Aβ42, Aβ40 and their 1:1 mixtures using thioflavin T (ThT) assay and electrospray ionization mass spectrometry (ESI-MS). Then, we further investigated the changes in gas-phase structures of homo- and hetero- oligomers of Aβ40 and Aβ42 using ion mobility spectrometry (IMS) combined with ESI-MS. Our results suggest that Aβ40 delays the nucleation process of Aβ42 by forming the hetero-oligomers, and overall rates in the fibrillation kinetics are decreased.

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발표분야: 분석화학
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확산이 제한된 하이드로젤 입자 내에서 핵산증폭반응 효율연구

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분자 수준에서의 진단에 대한 수요가 높아지는 가운데 임상적으로 가장 많이 사용되는 real-time PCR 은 실시간으로 유전자를 증폭하며 검출할 수 있으며, 정성· 정량 분석이 가능하다는 장점을 가진다. 반면에 한정된 수의 유전자만을 진단할 수 있기에 다중 진단 기술로서는 한계를 갖는다. 이를 극복하기 위해 Polyethylene Glycol(PEG)로 이루어진 입자 기반 real-time PCR 방법이 개발되었다. 이는 각기 다른 primer 를 고정시킨 입자를 이용하므로 여러 입자를 쓰면 한꺼번에 다양한 질병에 대한 진단이 가능하다. [1]
그런데 입자 내 에서의 분자 거동은 확산을 방해하는 입자 내 고분자 네트워크 때문에 용액 상에서의 분자 거동과는 상이한 양상을 보일 것으로 예상된다. 이런 입자 내에서 증폭 산물의 길이에 따른 반응 효율에 대한 연구가 보고되지 않았다. 본 연구는 다양한 길이의 증폭 산물을 만들 수 있도록 DNA template 와 primer 를 제작하여 액상과 입자 내에서의 증폭과 그 효율을 비교하고, 이를 개선하기 위한 방법을 제시하고자 한다. 표적 핵산의 정확한 정량적 정보를 얻기 어려워, 계열희석법을 이용해 각각의 template 길이 별 PCR 효율 및 입자간 균일성을 확인하였다.
Housekeeping gene 으로 잘 알려진 Beta actin 의 기존에 알려진 염기서열 일부를 중복하여 합성함으로써 70bp 에서 200bp 까지 template 를 제작하였으며, 그보다 더 긴 길이의 template 를 제작하기 위해 M13KE vector 에 각기 다른 primer 를 이용하여 증폭 산물의 길이를 150bp 에서 1000bp 까지 조절하였다. 계열 희석법을 이용해 정량적 분석을 한 결과 증폭산물의 길이가 200bp 이내에 대해서는 입자 내에서 PCR 효율이 90%이상으로 안정적으로 진행되었다. 500bp 와 1000bp 에서 액상 반응과는 달리 입자간 균일성이 떨어지고,

PCR 효율이 낮아지는 것을 확인하였다. 추가적으로 annealing 시간과 입자 내 다공성을 조절함으로써 1kb 수준의 template 에 대해서도 원활하게 PCR 이 진행되는 조건을 탐색중이다. 이 연구를 통해 다양한 표적핵산에 입자 PCR 적용이 확장될 것으로 기대된다.

[1] S. Jung et al., “Extensible Multiplex Real-time PCR of MicroRNA Using Microparticles ”, *Scientific Reports* , **6**, 22975, 2016

Key words: 실시간 중합효소연쇄반응 (real-time PCR), 수화겔 (hydrogel), 증폭산물의 길이, PCR 효율.

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Quantitative Analysis and Mapping Neuronal Proteins Using Atomic Force Microscopy

이동규 박준원[1,*]

POSTECH 융합생명공학부 [1]POSTECH 화학과

Proteins perform a vast array of functions within living organisms, including catalyzing metabolic reactions, DNA replication, responding to stimuli, and transporting molecules from one location to another. Detection of proteins of low expression level is frequently important, because a certain proteins exist at very low level during the early stages of cell development. In particular, neuronal proteins of the kind play a key role in the regulation of development and synaptic plasticity of neurons. Conventional methods to analyze proteins include western blotting, ELISA, and immunofluorescence. However, these tools suffer from poor limit of detection, and cannot visualize proteins in high lateral resolution. Therefore, atomic force microscopy (AFM) is a good candidate to overcome the hurdles. AFM is a powerful tool to get an image of the surface. Moreover, by using the AFM it can show information about the distribution of the biomolecule. Using the mapping capability and imaging mode of AFM, it is possible to obtain an image of a single neuron and map the distribution of a specific protein in a nanometeric resolution. In the congress, we present our effort to demonstrate such capability of AFM.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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Surface Structure of Amyloid beta Oligomers and Fibrils Analyzed by Atomic Force Microscopy

윤지현 박준원*

POSTECH 화학과

Atomic force microscopy (AFM) can image topography of biomolecules with the sub-nanometer resolution. Furthermore, since AFM imaging can be performed in an aqueous solution, it has been applied under physiological condition. AFM is also used to measure the interaction strength of biomolecules with the pico-Newton resolution. Based on the AFM imaging mode and force measurement, we can image the distribution of interaction site on sample with high spatial resolution and sensitivity. Here, we investigated amyloid beta (Aβ) oligomers and fibrils that are believed to play important roles in Alzheimer’s disease (AD) by using AFM force mapping mode.AD is one of the most prevalent severe degenerative neuronal diseases afflicting our elderly population. AD is characterized by synapse and neuron loss in the brain, the accumulation of senile plaques which are protein deposits, and neurofibrillary tangles. The Aβ is believed to play important causal roles in AD. Although many investigators studied such neurotoxic Aβ, the molecular structure of them remains unclear. We employed AFM to elucidate the surface structure of Aβ. Observed specific interaction between Aβ and both C/N-terminal specific antibody suggests a surface structure model in which both N-terminus and C-terminus are exposed at the surface.

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Visualization of MicroRNA Distribution in a Neuronal Cell Using Atomic Force Microscopy

박익범 구현서[1] 박준원[1,*]

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MicroRNAs (miRNA) are a class of short (~ 22 nt) noncoding single-stranded RNA that subserve post-transcriptional modulation. Especially, specific miRNAs of brain have important roles in neuronal differentiation, development, plasticity and induced neurological disorders. Visualization of miRNAs has emerged as an important topic in biomedical fields. Therefore, accurate visualization of miRNAs at the single-cell level is of great interest due to their heterogeneity among cell population. Conventional methods widely used in the detection of miRNAs mainly include northern blotting, microarray, real-time RT-PCR and in-situ hybridization. Especially, In situ detection of intracellular miRNAs requires simple sample preparation, without cell lysis and RNA isolation, and provides additional information on the subcellular localization of miRNAs. However, conventional tools are not easy to detect high spatial localization and sensitive detection of miRNAs. Therefore, a new approach for miRNA detection tool is atomic force microscopy (AFM). AFM has been extensively used to observe interaction of molecules and manipulate biomolecules in the physiological conditions at the single-molecule level. Because AFM has high lateral resolution of sub-nanometer, the nanoscale distribution of individual molecules on the sample surface could be imaged. Here, we established an AFM-based miRNA quantification and distribution method with no requisite of labeling for modification of miRNAs. In this research, visualization of a specific miRNAs in a cultured neuronal cell is measured by force-based AFM and help to understand functions of miRNA in depth.

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Supersensitive Analysis of MicroRNA Using Metal-Enhanced Fluorescence Nanoparticles

박수현 남좌민[1] 박준원*

POSTECH 화학과 [1]서울대학교 화학부

MicroRNAs(miRNAs) are known to be involved in protein transcription, physiological mechanisms such as development, differentiation, cell proliferation and apoptosis. They are also known to be associated with many diseases such as cancer, Alzheimer's disease, myocardial disease. miRNA is 22mer shorter than general RNA, thus miRNA is amplified by PCR. In particular, the role of miRNAs in cancer has been extensively studied. miRNA analysis can be useful for early diagnosis or treatment of diseases. Currently, Polymerase Chain Reaction (PCR) is a standard method to detect miRNA. However, it causes error in amplification process several times and analysis sensitivity is relatively low. In order to overcome the limitations of the conventional technology, I will improve the sensitivity more than 100 times by the fusion of fluorescence enhanced nanoparticles and microarray. Here we suggest new approaches to supersensitive analysis of miRNA using metal-enhanced fluorescence (MEF) nanoparticles and microarray. To detect miRNA, we use S9.6 antibody that is DNA/RNA hybrid-specific mouse monoclonal antibody. This approach is expected to perform parallel analysis with detection sensitivity increased several hundred times more than the conventional methods.Reference1. Z. Hu, et al. Nucl. Acid Res. 2006, 34, e522. B. J. Hong, et al. Nucl. Acid Res. 2005, 33, 12

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

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발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Replication and Transcription of Methylated DNA Studied with Atomic Force Microscopy

이지윤 박준원*

POSTECH 화학과

DNA methylation is one of the epigenetic mechanism that controls the function of genes without changing the genetic code. It is known that methylated DNA performs not only important genetic roles in normal cells, but also tumor cells. In cancer tissues, DNA methylation has been observed differently from normal cells, and the degree of DNA methylation in cancer tissues are thought to be epigenetic rather than genetic causes. Atomic force microscopy (AFM) have the capability of measuring intermolecular forces at the pico-Newton level while scanning surfaces at the nanometer resolution. AFM force spectroscopy has been used to observe molecular interaction and dynamics at the single-molecule level. Here, we show a study method of methylated DNA using AFM. In our approach, a DNA polymerase (DNAP) or RNA polymerase (RNAP) was immobilized on an AFM tip. The DNAP was allowed to capture a duplex of primer/template DNA and the RNAP was allowed to capture a initiator site of template DNA. Specific rupture events arising from the binding of complementary bases to the DNA/DNAP and DNA/RNAP complex were observed on the nucleotide-immobilized glass slide. Through this study, we propose to identify differences in DNA methylation during DNA replication and transcription process using polymerase and investigate the degree of binding between the target DNA and its complementary base at the reactive site of the polymerase during the polymerization. It is expected that the current method would enable the DNA methylation to be studied at the single cell level.

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발표코드: **BIO.P-274**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

염소 수처리에서 MRSA와 mecA gene 비활성화 효율

최예균 이윤호*

GIST 지구환경공학부

1. Introduction 전 세계적으로 항생제 내성균 및 내성유전자가 다양한 수계에서 검출되고 있다. 항생제 내성 증가는 인류의 건강을 위협하는 심각한 공중보건 이슈이다. 특히 항생제 내성물질의 존재가 세균 군집의 전체적인 항생제 내성의 증가를 야기할 수 있다는 연구 결과도 나옴에 따라 내성균 및 유전자의 환경 거동과 전파를 차단할 수 있는 환경 기술 개발에 관심이 높다. 본 연구에서는 수처리에 소독목적으로 널리 사용되는 염소 수처리에서 대표적인 항생제 내성균의 하나인 Methicillin Resistant Staphylococcus Aureus (MRSA)와 해당 내성균이 가지고 있는 mecA gene 내성유전자에 대하여 비활성화 효율을 측정하였다. 해당 내성균과 내성유전자 각각에 대해 염소에 의한 불활성화 반응속도를 측정하고 반응성 예측 모델을 구축함으로서 전통적 염소 소독수처리에서 어느 정도 수준까지 MRSA 와 mecA gene 이 비활성화 되는지 평가하고자 한다.2. Materials and Methods 본 연구에는 Gram(+)에 속하며 SCC mec gene cassette IV 내에 mecA 내성유전자를 Transposon 형태로 지니고 있는 ATCC BAA1556 가 MRSA 의 대표균주로를 선택되었다. 실험실 염소처리는 고농도 염소 stock 을 만든 후, 적정량을 희석하여 회분식 반응기에서 MRSA 및 S 내성유전자를 염소 주입량 혹은 반응시간에 따라 처리하였다. 염소 처리 후 Culture-dependent 한 plate counting 기법과 함께 Culture-independent 한 분자생물학 분석 기술 (Flow-cytometry, qPCR)을 이용하여 MRSA 및 mecA gene 불활성화 정도를 분석하였다.

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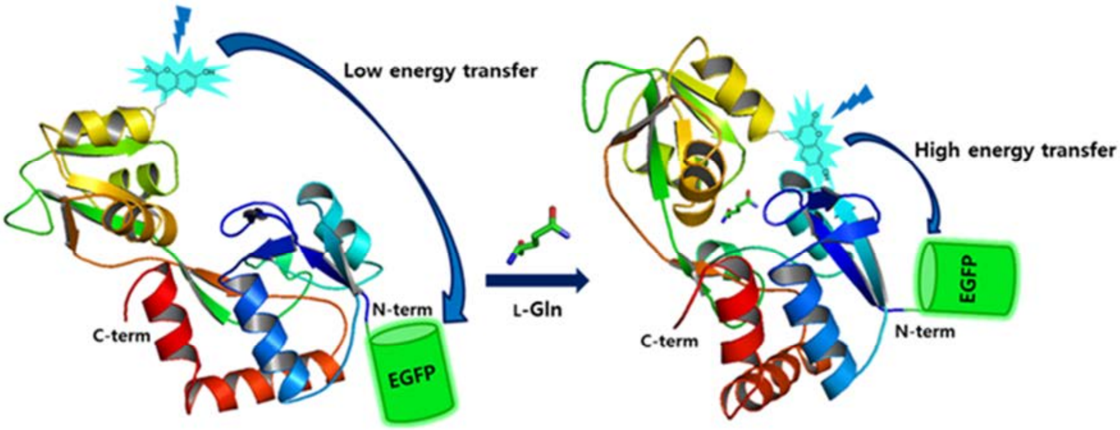
Genetically encoded FRET sensors using a fluorescent unnatural amino acid as a FRET donor

고우석 이현수*

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 study, 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
EGFP
C-term
N-term

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Direct protein-protein conjugation by genetically introducing bioorthogonal functional groups into proteins

김상길 이현수*

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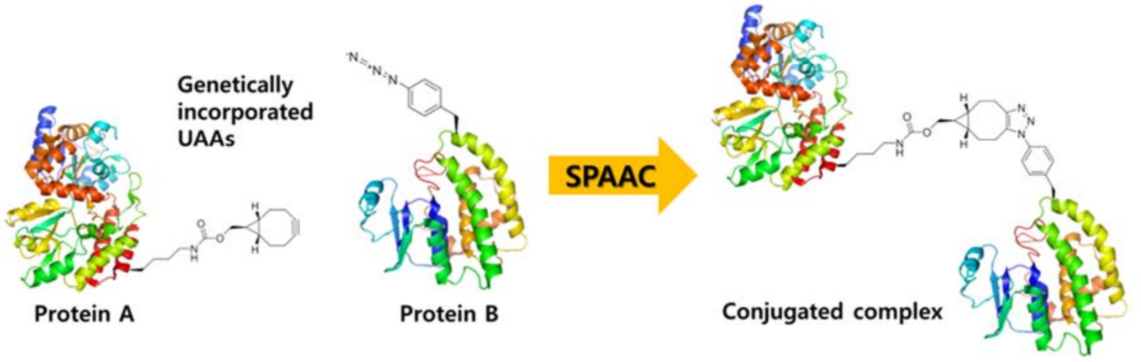
Proteins often function as complex structures in conjunction with other proteins. Because these complex structures are essential for sophisticated functions, developing protein–protein conjugates has gained research interest. In this study, site-specific protein–protein conjugation was performed by genetically 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 the 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 may prove very useful for generating protein–protein conjugates and protein complexes of biochemical significance.



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발표코드: **BIO.P-277**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Combining suppression of stemness with lineage-specific induction leads to conversion of pluripotent cells into functional neurons

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Sox2 is a key player in the maintenance of pluripotency and stemness, and thus inhibition of its function would abrogate stemness of pluripotent cells and induce differentiation into several types of cells. Herein we describe a strategy, which relies on a combination of Sox2 inhibition with lineage-specific induction, for promoting efficient and selective differentiation of pluripotent P19 cells into neurons. When P19 cells transduced with Skp protein, an inhibitor of Sox2, are incubated with a neurogenesis inducer, the cells are selectively converted into neurons which generate depolarization-induced sodium currents and action potentials. This finding indicates that the differentiated neurons are electrophysiologically active. Signaling pathway studies lead us to conclude that a combination of Skp with the neurogenesis inducer enhances neurogenesis in P19 cells by activating Wnt and Notch pathways. The present differentiation protocol could be valuable to selectively generate functionally active neurons from pluripotent cells.

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Synthetic ion transporters were based on calixpyrrole that perturb cellular chloride ion homeostasis induce caspase mediated apoptosis

박성현 신인재*

연세대학교 화학과

Synthetic ion transporters have received great attention as therapeutic agents because of their potential to perturb cellular ion homeostasis. However, a direct correlation between a change in cellular ion concentration and cytotoxicity has not been established for synthetic ion carriers. Herein we show that two pyridine diamide-strapped calix[4]pyrroles induce coupled chloride anion and sodium cation transport in both liposomal models and cells, and promote cell death by increasing intracellular chloride and sodium ion concentrations. Removing either ion from the extracellular media or blocking natural sodium channels with amiloride prevents this effect. The results of cell experiments indicate that the ion transporters promote the sodium chloride influx, which results in an increased concentration of reactive oxygen species, release of cytochrome c from the mitochondria and apoptosis via caspase activation. However, they do not activate the caspase-independent apoptotic pathway associated with the apoptosis-inducing factor. The present study suggests that artificial ion transporters represent an attractive approach for modulating cellular processes that are normally controlled tightly by homeostasis.

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Synthetic ion transporters were based on squaramide that disrupts autophagy and induces apoptosis by perturbing cellular ion homeostasis

박성현 신인재*

연세대학교 화학과

Perturbations in cellular chloride concentrations can affect cellular pH and autophagy and lead to the onset of apoptosis. With this in mind, synthetic ion transporters have been used to disturb cellular ion homeostasis and thereby induce cell death; however, it is not clear whether synthetic ion transporters can also be used to disrupt autophagy. Here, we show that squaramide-based ion transporters enhance the transport of chloride anions in liposomal models and promote sodium chloride influx into the cytosol. Liposomal and cellular transport activity of the squaramides is shown to correlate with cell death activity, which is attributed to caspase-dependent apoptosis. One ion transporter was also shown to cause additional changes in lysosomal pH, which leads to impairment of lysosomal enzyme activity and disruption of autophagic processes. This disruption is independent of the initiation of apoptosis by the ion transporter. This study provides the first experimental evidence that synthetic ion transporters can disrupt both autophagy and induce apoptosis.

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A Sirtuin 1 selective inhibitor induces neuronal differentiation of pluripotent P19 cells

이창희 신인재*

연세대학교 화학과

Sirtuin 1 (SIRT1), a histone deacetylases, is known to play important roles in neuronal differentiation of pluripotent / multipotent stem cells by regulating expression of neuron-associated genes. Several inhibitors of SIRT1 have been exploited for use in diverse biological functions, however, most of these inhibitors also known to function on other Sirtuin family proteins. Herein, we employed a potent and selective small molecule inhibitor of SIRT1 to test whether inhibition of SIRT1 activities can lead to the differentiation of P19 cells into neurons. In this effort, P19 cells were treated for 9 days with the selective inhibitor of SIRT1, EX-527, and then performed immunocytochemical, western blot and RT-PCR analyses. The results showed that EX-527 promotes neuronal differentiation of P19 cells without differentiation into astrocytes and cardiac cells. The findings indicate that the inhibitor induces selective neurogenesis of P19 cells. In addition, the differentiated neurons from P19 cells treated with EX-527 generated voltage-dependent sodium currents and depolarization-induced action potentials. These findings clearly indicate that the neuron-like cells have electrophysiological properties. The present study suggests that SIRT1 selective inhibitors could have the potential as chemical inducers to differentiate pluripotent cells into functional neurons.

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장소: 일산 KINTEX
발표코드: **BIO.P-281**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

HSP70 and HSC70 ATPase activity inhibiting small molecule that promotes immune response against protein antigens

박상현 신인재*

연세대학교 화학과

Number of biological processes is known to govern by the ATPase activities of Hsp70 and Hsc70, however, their roles on immune responses to antigens have remained largely unaddressed. In this study, the effect of apoptozole (Az), an inhibitor of Hsp70 and Hsc70, on immune responses to protein antigens was investigated. The results show that more antibodies produced when mice were treated with both protein antigen and Az compared to sole antigen treatment. This result indicates that Az exerts enhanced responses to administered antigens. The results of in vivo studies show that Az produced high titer of IgG2c/IgG1 antibodies with the concomitant release of Th1 and Th2-type cytokines. This finding indicates that Az activates the Th1 and Th2 immune responses. Taken together, the present study suggests inhibition of Hsp70 and Hsc70 can be an innovative way to provide small-molecule based adjuvants for protein vaccines.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.P-282**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

NMR Study on Structure of *Propionibacterium acnes* Acyl Carrier Protein by using NMR Spectroscopy

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건국대학교 생명공학과 [1]건국대학교 생명특성화대학

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. However, the structure of *P. acnes* ACP has not been studied yet. 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. Chemical shift index showed that *P. acnes* ACP has four α-helices (α1 (I7-T19), α2(S40-F54), α3(D60-N65), and α4(V69-H79)). Using chemical shift perturbation data upon the conversion by covalent modification by a phosphopantetheine prosthetic group, large chemical shift changes near the prosthetic group binding site at Ser40 and the residues (D39, L41, M43, E45, I46, E57, I58) forming a hydrophobic cleft. Using CD spectra, the melting temperature of *P. acnes* ACP was determined as 61.7°C, which is much lower than those of other ACPs, implying its low thermostability. We performed homology modeling on *P. acnes* using structure of *E.coli* ACP as a template and the results agrees well with the chemical shift index data. In our further study, we will determine three-dimensional structure of *P. acnes* ACP and study it dynamics. Based on these data, we will design inhibitors of FAS protein as a novel antibiotic against *P. acnes* infection.

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Comparison of Type I and Type II Acyl Carrier Protein using NMR Spectroscopy

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The synthases of Type I FAS are arranged as large multi-domain polypeptides. Acyl Carrier protein (ACP) is an acidic protein which is essential for fatty acid synthesis (FAS). In this work, Type I Human ACP and *S. coelicolor* ACPS were cloned, expressed, and purified. CD spectra of Human ACP showed double minima at 205 and 222 nm, which are characteristic of an α-helical structure. We performed multi-dimensional heteronuclear NMR experiments on 15N and 13C labeled protein and completed the backbone assignment. Chemical Shift Index showed that Human ACP has four α-helices, showing that α_1 and α_4 are relatively shorter compared to those of bacterial ACPs. Chemical shift perturbations upon conversion of the apo to the holo ACP, and octanoyl ACP revealed that Human ACP does not sequester growing acyl chain in the hydrophobic pocket. The hydrophobic triad residues in human ACP blocks the entrance to a hydrophobic pocket. The melting temperature of Human ACP is much higher compared to that of *E.coli* ACP and it was more stable in the absence of metal ion. Human ACP has more positively charged residues compared to bacterial ACPs which reduced the electrostatic repulsions. Since charge distribution of Type II FAS is different from that of Type I FAS, this makes bacterial FAS proteins as attractive targets for development of potent antibiotics.

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발표분야: 생명화학
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Backbone-modified oligonucleotides for tuning the cellular uptake behaviour of spherical nucleic acids

김경란 안대로[1,*]

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Spherical nucleic acids (SNAs) are spherically arranged oligonucleotides on core inorganic nanoparticles and have great potential for intracellular delivery of bioactive molecules, since they have been found to be internalized into mammalian cells. Understanding the factors that influence the cellular uptake of SNAs would be beneficial to design SNAs with novel uptake properties. We here report the effect of the sugar backbone type of the oligonucleotides on the cellular internalization of SNAs. After the preparation of SNAs with the oligonucleotides of five different sugar backbones, we analyze the cellular uptake efficiency quantitatively by flow cytometry and inductively coupled plasma mass spectrometry (ICP-MS). The data reveal that the uptake efficiencies and the uptake mechanisms significantly rely on the backbone type. These results suggest that the backbone modification can provide a unique handle to tune the cellular uptake behavior of SNAs.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Detection of cell signaling molecules using live cell-based sensing systems

전현진 권영은*

동국대학교 의생명공학과

Biological signal molecules transmit information between cells in vivo and play key roles in modulating cell metabolism, functions, and development. Detecting signaling molecules in living cells is important for understanding their roles in biological systems and for studying various disease-related mechanisms. Herein, we describe a genetically encoded fluorescent sensor based on fluorescent trans-localization by intein-mediated reactions. The approach utilizes the generation of functional signal peptide by intein-mediated splicing or cleavage reaction which is activated in response to external stimuli. We first tested the concept of fluorescent trans-localization sensor by using a pair of split-inteins which react spontaneously. Then a model system was prepared to monitor the rapamycin induced hetero-dimerization of FKBP and FRB. Additionally, we constructed a live cell based sensing system to monitor the influx of Ca2+, an important intracellular signaling molecules related to various cellular events, using calmodulin and calmodulin binding domain conjugated split-intein system. The sensing system successfully reported the change of intracellular Ca2+ levels induced by ionophore or histamine. Finally, the sensing of corticosterone, which affects various physiological responses such as gluconeogenesis, deposition of hepatic glycogen, and anti-inflammatory response, was also carried out using glucocorticoid receptor protein. This self-replicable live cell-based sensing systems can be engineered to report various cellular events of interest in biologically relevant environment thus can be used for drug screening and disease mechanism study.

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Small Angle X-ray Scattering Studies on Structures of Biological Macromolecules in Solution

진경식

POSTECH 포항가속기연구소

The fundamental aim of structural studies in molecular biology is to establish a relationship between the structure (or, more precisely, structural changes) and function of biological macromolecules. Over the past years, a tremendous amount of structural information has been obtained using macromolecular crystallography and nuclear magnetic resonance (NMR). These high-resolution methods apply only in rather specific conditions: it is often difficult to grow crystals of high molecular weight (MW) assemblies that are suitable for diffraction, and the application of NMR is fundamentally limited to small (MW < 30 kd) proteins. Investigation of structure of biological macromolecules in solution remains one of the most important fields of application of small angle X-ray scattering (SAXS) technique. SAXS permits analysis of biological macromolecules and their complexes in nearly physiological environments and direct study of structural responses to changes in physical and chemical conditions. Recent remarkable progress in instrumentation, in particular thanks to high-flux dedicated X-ray synchrotron radiation has significantly improved the quality of the experimental SAXS data. This method is an important complementary tool to the high-resolution techniques (X-ray crystallography and NMR). The fundamental aim of this study is to obtain more detailed information on the structure and structural differences of a variety of biological macromolecules in solution under various conditions by using SAXS technique. Ultimately, the structural evidence presented here will contribute to a better understanding of relationship between structures of macromolecules and their function, from a biophysics point of view. In this talk, current status of 4C SAXS beamline, long-term plan for advanced beamline, SAXS data processing, overall parameters, and recent research results of biomacromolecules (DNA, protein) will be discussed in more detail.

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장소: 일산 KINTEX
발표코드: **BIO.P-287**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Mechanistic study of O-ureidoserine racemase (DcsC)

안영찬

University of Alberta Chemistry

O-ureidoserine racemase (DcsC) is a PLP-independent racemase involved in the biosynthesis of important antibiotic D-cycloserine.[1] Our goal is to elucidate the mechanism of this unusual epimerization by means of crystallization of the enzyme with a known optically pure inhibitor.[2] Alternatively mechanistic information can be achieved by crystallization of the racemic inhibitor with site-specifically mutated DcsC variants. This approach has been shown successful in proving the proposed epimerization mechanism for the highly homologous diaminopimelate epimerase (DapF, 40% homology).[3] With a crystal structure in hand we will be able to visualize the 3D geometry of the active site revealing how DcsC is able to significantly decrease the pka of the substrate thus enabling the proton abstraction under physiological conditions . 1 Uda et al. Antimicrob. Agents Chemother, 2013, 57, 2603-26122 Dietrich et al., Org. Biomol. Chem. 2012, 10, 2248-2254.3 B. Pillai et al., Proc. Natl. Acad. Sci. 2006, 103, 8668-8673.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-288**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of inner ear-targeted drug delivery system with phospholipid nanoemulsion

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The purpose of this study is to develop an inner ear-targeted drug delivery system with phospholipid nanoemulsion. To optimize particles, we varied charges or attached polyethylene glycol (PEG) for safety and efficiency. Anionic, neutral, cationic particles and cationic-PEG particles was fabricated. PEG was attached to induce long circulation inside perilymph by avoiding non-specific binding with proteins. The sizes of candidate particles were about 200 nm. First, their cellular uptake was observed in HEI-OC1 cell. In FACS analysis, cationic particles showed most intense fluorescence, and cation-PEG, neutral, anionic particles were followed. However, in artificial mucosa exam, fluorescence intensity inside mucosa and HEI-OC1 cells below the mucosa was highest in case of cationic-PEG particles and neutral particles. The overall results demonstrate that cationic particles showed highest cellular uptake during in vitro exams similar to the previous studies, but to permeate RWM and deliver a drug to hair cells after circulating perilymph, attaching PEG or using neutral particles seems favorable.

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장소: 일산 KINTEX
발표코드: **BIO.P-289**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Anti-Tuberculosis Activity of 3,6-Dihydroxyflavone and its therapeutic effect against lung inflammation

곽철희 김양미*

건국대학교 생명공학과

In a previous research, we revealed that 3,6-DHF can be a potent anti-tumor and anti-inflammatory material on specific cancer cells. In this study, we investigated the anti-mycobacterial effects of 3,6-DHF against Mycobacterium tuberculosis(Mtb) and its anti-inflammatory effects for the first time. Our results showed that 3,6-DHF had anti-mycobacterial effects on H37Rv Mtb, MDR(multi-drug-resistant) Mtb, and XDR(extensively-drug-resistant) clinical isolates. The MIC90 values , which mean the minimum inhibitory concentration for bacterial cell growth are 25, 100 and 100 g/ml respectively. Mtb initially affects the lung and then influences other organs through blood and lymph nodes by accompanying with a strong local inflammatory response. We also investigated the effects of 3,6-DHF on lipopolysaccharide(LPS)-stimulated human lung fibroblast MRC-5 cells. 3,6-DHF reduced mRNA levels of tumor necrosis factor- interleukin (IL)-6, IL-12, IL-1 and matrix metalloproteinase-1 and inhibited levels of phosphorylation of ERK1 in MRC-5 cells. These data indicate that 3,6-DHF could be developed as a potential antituberculosis molecules and effectively reduced lung inflammation.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.P-290**

발표분야: 생명화학

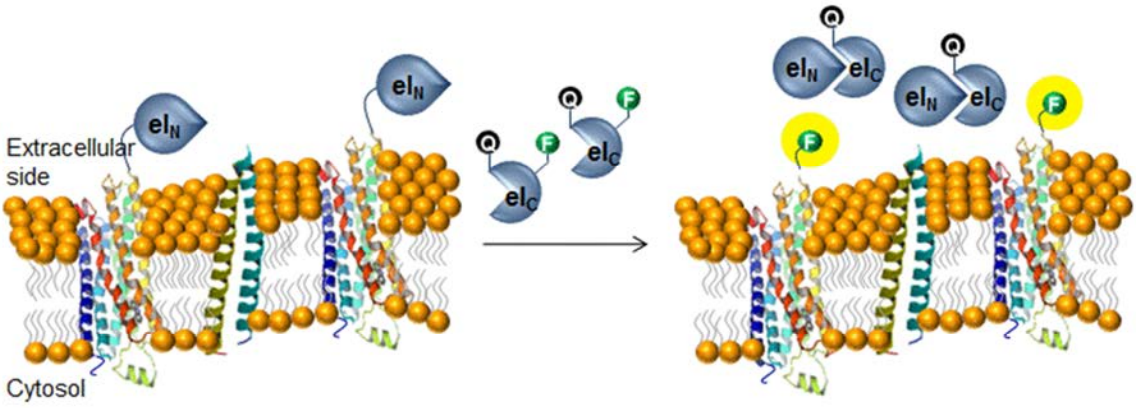
발표종류: 포스터, 발표일시: 금 13:00~14:30

Efficient labelling of membrane proteins using engineered Npu DnaE split-inteins

이의연 권영은*

동국대학교 의생명공학과

Membrane proteins are the most abundant of whole proteome in mammalian cells and they play core roles in regulating cellular events. Membrane proteins also are good drug targets and it is important to monitor their dynamics and trafficking. Spectroscopic monitoring of proteins in living cells is a critical tool in cell biology as it allows non-destructive real-time observation of protein functions, interactions, and trafficking in their native context. However, as most proteins are not spectroscopically active it is desirable to introduce a spectroscopic tag to a target protein specifically in live cells. Here, we present a method to label membrane protein of interest based on split-intein mediated protein trans-splicing (PTS) reaction. A pair of engineered Npu DnaE were utilized for efficient labeling membrane protein on living cells. The labeling reaction occurred in two sequential reactions, namely via specific binding of two split-intein fragments followed by covalent conjugation through split-intein mediated PTS reaction. The specific binding occurred instantly and the covalent labeling was observed in 5 min on live cells with minimal background staining. This approach can be used as a tool to monitor the trafficking of membrane proteins and cell signaling events.


Extracellular side
Cytosol
eI$_N$
eI$_N$
Q
F
eI$_C$
Q
F
eI$_C$
Q
eI$_N$
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Q
eI$_N$
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F
F

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장소: 일산 KINTEX
발표코드: **BIO.P-291**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The kinetics studies on protein trans-splicing reaction based on electrostatic potential of exteins

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Protein trans-splicing (PTS) reaction is self-processing reaction mediated by a pair of split-inteins. PTS-based protein semi-synthesis is widely used for conjugation of various synthetic probes to target proteins *in vivo* and *in vitro*. As PTS reaction became a useful tool for various biological studies, it is important to understand the factors that affect the kinetics of PTS. Previously, there are a number of reports describe the roles of penultimate residues of inteins and the key amino acids of N- and C-exteins, usually the immediately flanking sequences, for ensuring the PTS activity. However, we also observed the PTS rates varied in large extend depending on the proteins that are used as exteins, even when the penultimate residues and immediate flanking sequences are well maintained. And there is no reasonable explanation offered for this variation yet. As there is an enormous complexity of all possible flanking sequences, we analyzed how the electrostatic potentials of flanking sequences affect PTS kinetics. For this study, we have chosen a fast reacting ($t_{1/2}$ ~1 min) and naturally split-Npu DnaE intein as a model system. We prepared multiple pairs of split-inteins that carry exteins of various pI's and analyzed the kinetics of *in vitro* PTS reactions. We observed that the higher pI value of N-intein flanking sequences (N-flanking) and lower pI value of C-intein flanking sequences (C-flanking) accelerated PTS reaction. We also confirmed this result using PTS reactions on live cells. A model cell surface protein was fused to N-intein and reacted with two fluorescent C-inteins. The C-intein carrying an extein with lower pI mediated faster labeling reaction. This study offers a good guideline in designing fast reacting PTS system.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-292**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Biological effect of modified AuNPs depending on the surface charge and ligand structure

고종연 이의연 권영은*

동국대학교 의생명공학과

AuNPs are widely utilized for numerous biomedical applications as they exhibit superior biocompatibility and marginal toxicity. AuNPs can be modified to obtain various physic-chemical properties and it is important to understand how the physico-chemical properties of AuNPs affect their biological interactions. Among many variables, we here focused on the effect of surface chemistry, i.e. charge and structure of ligands. For a systematic approach, we prepared mono-dispersed AuNPs carrying various functional groups based on a sequential ligand exchange method. The prepared AuNPs had surface charges ranging from -36.1±1.4 mV to +37.1±0.5 mV. Various biological assays were performed to measure the effects of each AuNPs on cell viability as well as on various cellular functions. Uptake efficiency of AuNPs by mammalian cells and the subsequent changes of cell morphologies and cytoskeletal structures were also monitored. These studies showed that the cytotoxicity of anionic and neutral AuNPs were insignificant, whereas cationic AuNPs showed mixed effects from non-toxic to severely toxic, depending on the structure of ligands. While all the cationic AuNPs tested were more effectively internalized by mammalian cells compared with anionic or neutral AuNPs, only the cytotoxic MUAM-AuNP showed inhibitory effects on the DNA replication and on the formation of actin filament. The results showed that not the charge of the AuNPs but the structure of the ligand was an important factor determining the biological effects of AuNPs. This work also proposed that properly designed cationic AuNPs could make a good candidate for low toxicity gene-delivery materials.

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장소: 일산 KINTEX

발표코드: **BIO.P-293**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Studies on distinguishment of various influenza virus subtypes by counter systematic evolution of ligands by exponential enrichment

이태균 정용주*

국민대학교 생명나노화학과

Flu is caused by infection from influenza virus and brings symptoms like cold. Influenza virus contained single-stranded RNA. If this disease is transmitted to human by poultry, the situation becomes serious. There are many subtypes in influenza virus depending on the kinds of hemagglutinin (HA) and neuraminidase (NA). HA is a surface protein of influenza virus, and this is involved in the viral infection by binding the sialic acid of the host cell. All subtypes of influenza virus have different types of HA. So we have tried to find molecular probes that specifically bind to each different HA for diagnosis of the various influenza virus. To find the probes, we have applied the counter systematic evolution of ligands by exponential enrichment (Counter-SELEX) method. Then, we measured the binding affinity of the probes by enzyme-linked immunosorbent assay. We expect the probes will be helpful to distinguish the various types of HA and diagnose influenza virus.

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fluorescent Carbon dots using Bisphosphonate derivatives for Bioimaging

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한국생명공학연구원(KRIBB) 위해요소감지BNT연구단 [1]과학기술연합대학원대학교(UST) 나노바이오공학과 [2]전남대학교 대학원 고분자공학과 [3]한국생명공학연구원 바이오나노연구센터

Abstract We synthesized hydrothermally water-soluble BP-CDs(Bisphosphonate-based carbon dots) using commercial osteoporosis medicines such as Alendronate, Zoledronate, Ibandronate and Risedronate. BPs are used for osteoporosis treatment clinically and are good candidates as a bone-imaging agent because of high affinity for hydroxyapatite. CDs were made from BP derivatives as the source of carbon and 1,2-ethylenediamine as the surface passivation agent. We confirmed that they exhibited the highest fluorescence intensity at 400nm and good photo stability. Due to superior biocompatibility, BP-CDs were imaging in living HeLa cells, which indicated that it is applicable in various fields of bioimaging. The high affinity of BP-CDs for hydroxyapatite also were verified through α-TCP(Tricalcium phosphate) scaffold incubated in BP-CDs solution. As new fluorescent carbon material, advantages of BP-CDs include strong fluorescence, water solubility, low cytotoxicity and high affinity for hydroxyapatite. They are suitable candidates for the applications in the bioimaging field.

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Characterization of Middle East Respiratory Syndrome Coronavirus Helicase

표소희 정용주*

국민대학교 생명나노화학과

An infectious respiratory disease, Middle East Respiratory Syndrome (MERS), is caused by a modified coronavirus. MERS coronavirus is a (+) single stranded RNA virus. Of the several non-structural proteins produced from the virus, NTPase/helicase plays an important role in viral replication. Helicases are motor proteins that separate double-stranded nucleic acids using energy generated from ATP hydrolysis. In the present study, we purified a recombinant MERS coronavirus helicase and measured ATP hydrolysis rates in the presence of various kinds of nucleic acids. In addition, basic kinetic parameters were also obtained.

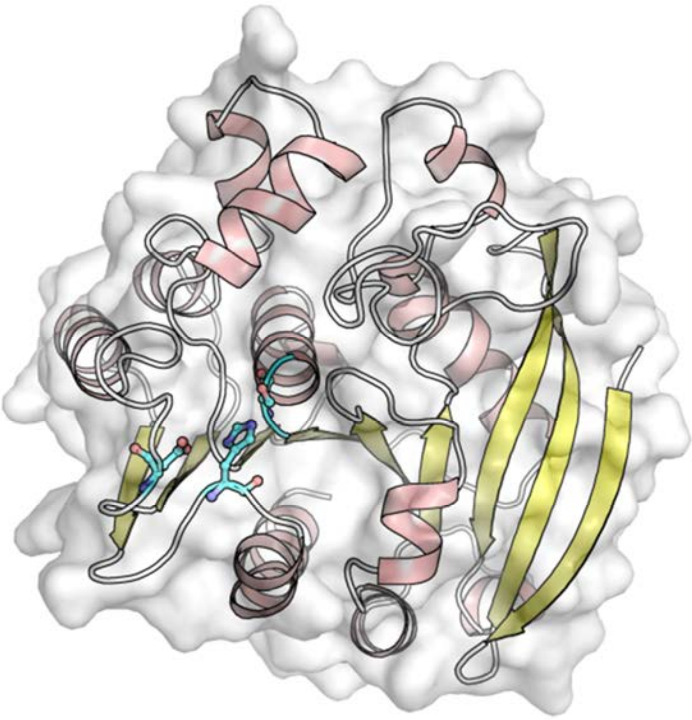
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-296**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Biochemical characterization of a novel esterase from an antarctic bacterium *Shewanella frigidimarina*

류범한 김두헌[1,*]

성균관대학교 의과대학/의생명과학과 [1]숙명여자대학교 이과대학 화학과

A novel esterase (Sf310) from Shewanella frigidimarina, which is composed of 279 amino acids with a molecular mass of 31.0 kDa, was identified, expressed and characterized. This enzyme displayed remarkable identity with S-formylglutathione hydrolases generally known as Esterase D family. Sequence analysis of Sf310 revealed a conserved pentapeptide of G-X-S-X-G found in various lipolytic enzymes and a putative catalytic triad of Ser148-Asp224-His257. Sf310 was active toward short-chain esters such as p-nitrophenyl acetate, butyrate, hexanoate and octanoate, while S148A mutant completely lost its activity. The optimum pH for enzyme activity was slightly alkaline (pH 8.0). Regarding the optimum temperature, interestingly, Sf310 could retain more than 80% of its full activity throughout temperatures ranging from 20 to 120 ℃, although circular dichroism spectroscopy showed that the enzyme is structurally thermolabile above 40 ℃.Moreover, Sf310 displayed above 50% of its initial activity with various chemicals including 30% EtOH, 1% triton x-100, 1% SDS, 5M urea and so on. Taken together, the high thermal and chemical stability of Sf310 could be useful for industrial application and give an insight into the stability of enzymes from Antarctic species.



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발표코드: **BIO.P-297**
발표분야: 생명화학
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Multi-functional nanocomposites for photodynamic therapy against tumor cells

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중앙대학교 화학과

For an advanced concept to theranostics, the integration of diagnostic and therapies has been attracted to much attention not only improving the treatment efficiency but also reducing the side effects. It can be realized by introducing the multifunctional nanocomposite, which can act as an imaging probe, drug delivery, and therapeutic effect itself. In this study, core-shell structured upconversion nanoparticles (UCNPs) and graphene oxide quantum dots (GOQDs) have been proved to be a target to the cancer cells. UCNPs have distinctive characteristics for diagnosis, and GOQDs have been widely studied as a promising drug delivery carrier to improve the tumor therapeutic effect. The UC luminescent techniques have been performed to verify apoptosis/necrosis of cancer cells. The UCNP-GOQD was conjugated by amine-PEG-carboxylic acid. In addition, hypocrellin A (HA) as a photo-sensitizer was loaded on the surface of GOQD by π-π interaction to enhance the anti-tumor effect. In order to show the enhancement of photo-dynamic therapy (PDT), different experiments were performed with free HA and UCNP-GOQD. In conclusion, the anti-tumor ability has been noticeably enhanced because of photodynamic tumor cell death based on the nanocomposites. Therefore, the UCNP-GOQD/HA nanocomposites would be excellent candidates as multifunctional agents for imaging and therapy.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **BIO.P-298**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Investigation of Oligomerization Process of Alpha-synuclein

배진의 김준곤*

고려대학교 화학과

Many human diseases arise from protein misfolding, in which neurodegenerative diseases such as Parkinson's disease (PD) are related to fibrillar aggregates called amyloid fibrils. Alpha-synuclein aggregates to form insoluble fibrils in pathological conditions such as Parkinson's disease. Alpha-synuclein which is found mainly at the tips of nerve cells (neurones) in the brain is a primary structural component of Lewy body fibrils. Although the oligomerization and further fibrillation of alpha-synuclein are critical factors in PD, the aggregation mechanism of alpha-synuclein is not clearly revealed. To understand the detailed process and compositional change of monomers, oligomers, and fibrils during the process, we performed quantitative and qualitative analysis at the same time. In quantitative analysis, matrix-assisted laser desorption ionization (MALDI)-MS and triple quadrupole-MS were performed. To avoid dissosication of oligomers into monomer during ionization process, cross-linking agents were adopted. In qualitative analysis, the conformational characteristics of the oligomers were investigated using ion mobility-mass spectrometry (IM-MS).

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-299**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Growth and development of *Suaeda glauca* through salt-defense mechanisms

이승재

전북대학교 화학과

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. The halophyte, *Suaeda glauca* (*S. glauca*), has many advantages in terms of biomass and saline elimination due to its large mass and well-developed phenotype on seashores, although its mechanistic features and growing specificities still require systematic investigation. Preliminary studies have indicated that secondary metabolites, including alkaloids, are key metabolites for achieving salt tolerance and that indole derivatives retard the inhibition of growth and development in halophytes. Metabolomic studies have validated that indole-3-carboxylic acid (ICA) and indole-3-acetic acid (IAA) accumulate in halophytes under saline conditions. In this study, *S. galuca* were cultivated under various saline concentrations (0–400 mM) in Hoagland's solution in the absence or presence of indoles to elucidate physiological features via systematic monitoring. The results confirmed that the optimal growth and development of*S. glauca* in 50 mM NaCl, and the morphology, such as the number of branches, shoot lengths, and fresh and dry weights, were improved by exogenous ICA treatment. The cation concentrations in roots, shoots and leaves were investigated to examine the ionic imbalance in response to saline treatment, and the results demonstrated that sodium ions accumulated to high concentrations in leaves. The levels of calcium and potassium ions in root were maintained at 50 mM NaCl, an optimal growth condition, but ICA and IAA did not regulate the ion concentrations. This study demonstrates the optimal growth conditions in saline for *S. glauca* and the phenotypic regulation of ICA, although the ionic imbalance was controlled by genetically programmed physiology. These results will provide valuable information for bioengineering based on the high levels of biomass in *S. glauca* to achieve salt tolerance in glycophytes and halophytes.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.P-300**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Paper chip-based simple, rapid, colorimetric detection of kanamycin using ssDNA aptamer

하나름 정인필 김아루 김상헌 윤문영*

한양대학교 화학과

Kanamycin is an one of the most important subclasses of aminoglycoside antibiotics which has been widely used to treat diverse infections. However, residual kanamycin can cause various side effects in humans such as loss of hearing, kidney toxicity. The risk of antibiotic residues in meat and milk is well known and focuses on intensive regulatory processes. Thus it is necessary to develop highly sensitive diagnostic kit for residual antibiotics. In this study, we developed the label-free AuNPs-based colorimetric aptasensors on paper chip. The 13 nm AuNPs were synthesized by citrate reduction of HAuCl4 and paper chips were designed and printed on LFNC 80 membrane using a wax-based printer. The citrate-coated AuNPs were modified with the 39 mer kanamycin binding aptamer for 15 min at RT with mild shaking. Then different concentration of kanamycin was added, and after the addition of high concentration of NaCl into the mixed solution. The visual results were monitored by naked eye and measured the delta RGB value. Kanamycin was detected until very low pM range within 30 min. In conclusion, the proposed system could accurately detect kanamycin and this results demonstrate the designed system could be applied for rapid detection of kanamycin in real samples.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **BIO.P-301**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Identification of potent inhibitors against Mycobacterium tuberculosis based on Acetohydroxyacid synthase (AHAS) inhibition

최재우 정인필 하나름 윤문영*

한양대학교 화학과

Mycobacterium tuberculosis acetohydroxyacid synthase (MTB-AHAS) was used as an important target for antimicrobial agents. We used high-throughput screening of a chemical library to find potent new inhibitors of MTB-AHAS. Among the 6800 tested compounds, 15 were identified as potent inhibitors, with an inhibition of in vitro MTB-AHAS activity of 80-90% at a fixed 20μl concentration. Five compounds similar to the triazolopyrimidine structure showed greater inhibitory potency, with a half-maximum inhibition concentration (IC50 value) in low micromolar range (0.4-1.24 [mu] M). Molecular docking of these inhibitors with MTB-AHAS showed that hydrophobic and hydrogen bond interactions with some key herbicide binding site residues with binding energies (ΔG) of −8.04 to −10.68 Kcal/mol, respectively. Importantly, These potent inhibitors demonstrated significant growth inhibition of various clinically isolated multidrug-resistant and extensively drug-resistant M. tuberculosis strains. In summary, the identified potent inhibitors have the potential to be used in future in vivo experiments or in the development of anti-bacterial agents against the more potent MTB-AHAS.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-302**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of a ssDNA aptamer to detect the Nonylphenol ethoxylate with Graphene oxide

김아루 하나름 정인필 김상헌 윤문영*

한양대학교 화학과

An endocrine disruptor is a major public health problem to people throughout the world. In the human body, the endocrine disruptors functionalize same as a sexual hormone with inducing a precocious puberty, gynecomastia, etc. Nonylphenol, one of the endocrine receptor, has attracted attention due to its prevalence in the environment and its ability to act with estrogen-like activity and it arises from the environmental degradation of Nonylphenol ethoxylates (NPEs), which is used to make detergents and it can also act as endocrine disruptor. So, NPEs should be detected easily and fast to prevent taking from laundry or dish and damaging caused by it and its metabolite.Herein, we developed a novel single strand DNA (ssDNA) aptamer for detection of NPEs. For this process, graphene oxide (GO) is used to gather unbound ssDNA with the counter target and GO-bound ssDNA is eluted with the target. We found aptamers and characterized with AuNP. Synthesized aptamers can bind to NPEs with high binding affinity. The aptamers have Kd value from tens of to hundreds of nanomolar (nM) level. Specificity of the aptamers also tested. One of them can distinguish specifically NPEs from the other chemicals We expect the aptamer can be a useful tool on a sensitive detection system towards NPEs for people's health.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-303**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Characterization and Immobilization of a novel esterase (LCK37) from *Leuconostoc citreum*

Wang Ying 김두헌[1,*]

숙명여자대학교 화학과 [1]숙명여자대학교 이과대학 화학과

A recombinant carboxylesterase (LCK37) from Leuconostoc citreum was cloned, over-expressed in Escherichia coli and characterized using biochemical methods. Sequence analysis of LCK37 revealed a putative catalytic triad (Ser170, Asp269 and His301). Based on phylogenetic tree analysis, it can be concluded that LCK37 is a member of new enzyme family with conserved catalytic motif GESSG. Biochemical properties of LCK37 were performed using mass spectrometry, circular dichroism (CD), fluorescence, gel filtration, kinetics, activity staining and pH indicator-based colorimetric assays. Two interesting mutations (L107A and W228A) completely lost their activities towards short-chain p-nitrophenyl (pNP) esters. Cross-linked enzyme aggregates (CLEAs) of LCK37 were prepared by precipitating the enzyme with ammonium sulfate and subsequent cross-linking with glutaraldehyde. Furthermore, Hybrid magnetic cross-linked enzyme aggregates (HM-CLEAs) of LCK37 were developed by co-aggregation of enzyme aggregates with magnetite nanoparticles and subsequent chemical cross-linking with glutaraldehyde. Remarkable stability and reusability of the HM-CLEAs of LCK37, highlight its potential as a biocatalyst in the pharmaceutical and chemical industries.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Identification of Mycobacterium tuberculosis Caseinolytic protease C1 (ClpC1) binding peptide and synthesis of ecumicin-CBP derivatives

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한양대학교 화학과

Caseinolytic protease C1 (ClpC1) in Mycobacterium tuberculosis (MTB) is a general stress protein which belongs to the heat shock protein 100 (hsp100) family of molecular chaperones. ClpC1 is a promising target for the development of new anti-tuberculosis agent, since ClpC1 have been identified as having a role in protein homeostasis in MTB strains. Ecumicin ClpC1 is one of the potent inhibitor for MTB based on the activation of ClpC1. In this study, we identified the ClpC1 binding peptide (CBP) by phage display. Among the identified peptide, 2 peptides (CBP1 and CBP2) exhibited similar binding and activation property to ecumicin. In order to increase the inhibition and permeability to MTB, CBPs were linked with ecumicin by esterification of Diepoxy butane. The size of synthesized derivatives was measured by MALDI-TOF and estimated to approximate 2.6 kDa consisted of 1.5 kDa Ecumicin and 1.1 kDa CBP. The synthesized derivatives exhibited ClpC1 activation property and inhibition against protease activity of ClpC1/ClpP1, P2 complex. This research might provide an impetus for the development of a strong anti-tuberculosis agent targeting MTB ClpC1.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-305**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Biochemical Characterization of a hormone sensitive lipase homolog (Lg36) from *Lactococcus garvieae*

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숙명여자대학교 화학과 [1]숙명여자대학교 이과대학 화학과

A novel oligomeric carboxylesterase (Lg36) from Lactococcus garvieae was identified, over-expressed in Escherichia coli, characterized, and immobilized for industrial application. Primary sequence analysis revealed that Lg36 has a catalytic triad consisting of Ser159, Asp256 and His286. Phylogenetic analysis showed that Lg36 was clustered in a branch of the family IV group. Biochemical properties of Lg36 were investigated by performing mass spectrometry, circular dichroism (CD), fluorescence, gel filtration, and pH indicator-based colorimetric assays. Furthermore, four important residues (F207, L208, F216, L258) involved in the formation of substrate-binding pocket were identified from structure analysis and mutagenesis. Cross-linked enzyme aggregates (CLEAs) of Lg36 were prepared by precipitating the enzyme with ammonium sulfate and subsequent cross-linking with glutaraldehyde. In addition, hybrid magnetic cross-linked enzyme aggregates (HM-CLEAs) of Lg36 were developed by co-aggregation of enzyme aggregates with magnetite nanoparticles and subsequent chemical cross-linking with glutaraldehyde. Interestingly, HM-CLEAs of Lg36 was enhanced in stability and recycling compared to CLEAs, which could be used for industrial application.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-306**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of novel imaging agent for alzheimer's disease using small peptide specific to amyloid beta

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Amyloid-beta 42 (Aβ42) is produced from proteolytic cleavage of the amyloid precursor protein (APP) and it is accumulated forming the many amyloid structures which are the main cause of Alzheimer's disease. For that reason, Aβ42 is known as a biomarker of AD. Here, we purified recombinant Aβ42 and confirmed the protein activity by making amyloid beta fibrils. Four different peptides (12mer) which bind to recombinant Aβ42 were screened via M13 phage display. The selected peptide shown micromolar range (μM) of binding affinity to target Aβ42. We verify the binding ability of peptide using immunoprecipitation-like methods immunofluorescence methods. Our protein is well precipitated using screened peptides. And high percent (>80%) of merging image were observed when the brain tissue (3X Tg-mouse) stained using peptide and antibody. Finally, to design a peptide based contrast agent, we conjugated Aβ42 specific peptides to the ultrasmall superparamagnetic iron oxide (10nm) through EDC/NHS coupling reaction. Such peptide based USPIOs that target neurotoxic accumulation of Aβ42 are potentially useful for early diagnosis of Alzheimer's diseases and disease management.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.P-307**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Characterization and mutational analysis of a cold-adapted bacterial lipase, SaHSL from *Salinisphaera sp. P7-4*

유완기 김부영[1] 김두헌[2,*]

성균관대학교 의과대학 [1]숙명여자대학교 화학과 [2]숙명여자대학교 이과대학 화학과

Hormone sensitive lipase (HSL) contributes energy metabolism and fatty acid signaling in various tissues. Functional and structural properties of HSL from human have been studied in detail, however, lipase homologues from bacteria are still largely unknown. Previously, a new cold-adapted bacterial lipase, SaHSL was identified and purified. Here, biochemical and biophysical studies of SaHSL were reported. Primary structure analysis of SaHSL revealed that SaHSL was different from human HSL, especially in N terminal region and regulatory domain. Here, SaHSL were investigated with fluorescence analysis, dynamic light scattering (DLS), electron microscopy, and time of flight (TOF) mass spectrometry. Studies of site-directed mutants in regulatory region suggested that the region are critical for structural stability as well as for substrate specificity. Improvement of chemical, thermal resistance and good durability of immobilized SaHSL proposed the potential as a biocatalyst in industries.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **BIO.P-308**

발표분야: 생명화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Characterization of a novel SGNH hydrolase (Nm21) from *Neisseria meningitidis 053442*

유완기 김부영[1] Wang Ying[1] 김두헌[2,*]

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Nm21, a novel SGNH-hydrolase from Neisseria meningitidis 053442 was identified, purified, and characterized by biochemical and biophysical methods. Multiple sequence alignment of Nm21 with other SGNH family member proteins confirmed a putative catalytic triad (Ser29-Asp169-His172), and conserved sequence motif of Ser(S)29-Gly (G)87-Asn (N)89-His(H)172. In this paper, biochemical properties of Nm21 were studied with fluorescence analysis, dynamic light scattering (DLS), electron microscopy, and time of flight (TOF) mass spectrometry. It was found that Leu92 residue neighboring catalytic cavity is responsible for stabilization of hydrophobic moiety in substrates, while at the same time it hinders the pathway of bulky substrates to get in the active-site pocket. At last, immobilization of Nm21 exhibited good durability after repeated usages and improved catalytic efficiency. Collectively, this study emphasizes a potential of Nm21 as a biocatalyst in the pharmaceutical and chemical industries and provide a deeper insight at substrate specificity of SGNH-hydrolase.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표종류: 포스터, 발표일시: 금 13:00~14:30

In situ simulation of pfEstA, a novel family VIII carboxylesterase, from *Pseudomonas fluorescens KCTC 1767*: a predictions of substrate selectivity through molecular modeling

유완기 김부영[1] **Wang Ying**[1] 김두헌[2,*]

성균관대학교 의과대학 [1]숙명여자대학교 화학과 [2]숙명여자대학교 이과대학 화학과

pfEstA, a novel family VIII carboxylesterase, is identified and analyzed in this study. Multiple sequence alignment and phylogenetic analysis confirmed that pfEstA is a member of family VIII carboxylesterase and a putative catalytic triad (Ser79-Lys82-Tyr168). Here, pfEstA was compared with other enzymes of the same family and Class-C β-lactamases which were retrieved from BLAST and DALI server. The computation simulation analysis of pfEstA with cephalothin and the result from hydrolysis of nitrocefin indicated that pfEstA would have little or no activity for hydrolysis of bulky β-lactam antibiotics. Structural analysis with other related enzymes and mutational study suggested that the structural individuality in the catalytic pocket elucidates the substrates selectivity of pfEstA rather than specific interaction between residues and substrates.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Hybrid immobilization with magnetic iron oxide nanoparticles of an Esterase (EaEST) from Exiguobacterium antarcticum

김부영 유완기[1] **Wang Ying** 김두헌[2,*]

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A novel immobilization of EaEST was performed by co-aggregation with magnetite nanoparticles (MNPs) and glutaraldehyde as cross-linking reagent. The hybrid aggregated EaEST with MNPs was analyzed by scanning electron microscopy and confocal laser scanning microscopy. In this study, the hybrid magnetic cross-linked EaEST (HM-EaEST-CLEAs) retained its activity by 70%, relative activity to soluble Ha28, over 18 cycles of reuse. HM-EaEST-CLEAs was analyzed by various biochemical methods for confirming the efficiency. Compared with free enzyme and standard CLEAs, the HM-EaEST-CLEAs exhibited high thermostability. And high stability also revealed in harsh states such as various pH levels and solvents. In addition, we carried out kinetics assay which was revealed the improvement of the immobilized efficiency. These characteristics make it promising as a biocatalyst for industrial processes.

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발표코드: **BIO.P-311**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A near-infrared fluorescent sensor with a self-immolative linker for the quantitative detection and imaging of hydrogen sulfide in vivo

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Hydrogen sulfide is a critical biological messenger, but few biologically compatible methods are available for its detection in vivo. Here, we describe the design and synthesis of a novel azide-functionalized near-infrared probe, NIR-Az, for a hydrogen sulfide assay in which a self-immolative linker is incorporated between the azide moiety and phenolic dihydroxanthene fluorophore from a cyanine dye. A large "turn-on" near-infrared fluorescence signal results from the reduction of the azide group of the fluorogenic moiety to an amine, in which the self-immolative linker also enhances the accessibility of NIR-Az to hydrogen sulfide. NIR-Az can select hydrogen sulfide from among 16 analytes, including cysteine, glutathione, and homocysteine. By exploiting the superior properties of NIR-Az, such as its good biocompatibility and rapid cell internalization, we successfully demonstrated its usefulness in monitoring both the concentrationand time-dependent variations of hydrogen sulfide in living cells and animals (detection limit less than 0.26 μM), thereby providing a powerful approach for probing hydrogen sulfide chemistry in biological systems.

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장소: 일산 KINTEX

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A sandwich immunoassay for detection of *Mycobacterium tuberculosis* secretory antigen using recombiant antibodies

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중앙대학교 화학과

Mycobacterium tuberculosis (*M.tuberculosis*) is a serious infectious pathogen causing tuberculosis (TB). Because it affects the lungs and spread easily through the air, TB has become a global threat leading people to deaths especially in developing countries. To prevent TB spreading and also improve patient care, rapid and accurate diagnosis method of TB is required for its early diagnosis. In this study, one of the secretory antigen of *M.tb* was chosen as a target for early TB diagnosis. Three different single-chain antibody fragments (scFv) against target were expressed in Escherichia coli. These antibodies were analyzed for its binding affinities with the target through SPR analysis. With these recombinant antibodies, a rapid and sensitive sandwich enzyme-linked immunosorbent assay (ELISA) for TB detection was developed. The antibodies fused to alkaline phosphatase (AP) was constructed, expressed and validated by the AP enzyme activities. Moreover, binding properties of AP-fused antibody with target was confirmed through colorimetric analysis and proved its efficiency as a detection antibody. With this, the sandwich ELISA was performed with wide-range concentration of target and the results showed high sensitivity and selectivity towards target proving its great potential as a TB diagnosing tool.

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Expression, purification and functionality of soluble ERLBD domain

윤소영* **이경희**

세종대학교 화학과

Discovery of destabilization domains (DDs) of estrogen receptor ligand binding domain(ERLBD, 297-549) have led us to investigate the regulatory role of these domains on fibril formation of amyloidogenic proteins, such as α-Synuclein (αSyn) as well as human islet amyloid polypeptide (hIAPP). For the purpose of overexpression and purification of soluble ERLBD, we have constructed the original plasmid $\text{ERLBD}_{297\text{-}549}$/ pET28a. Upon induction by IPTG, ERLBD was overexpressed in bacteria, but purification was not successful because of insolubility. Here, we compare the other domain construct ($\text{ERLBD}_{302\text{-}552}$) with $\text{ERLBD}_{297\text{-}549}$ in order to search for the optimized condition of purification. Functional role of $\text{ERLBD}_{302\text{-}552}$ on amyloid fibril formation is also discussed based on Thioflavin T (ThT) fluorescence.

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Studying effect of ECM on mechanical properties of artificial cells by micropipette aspiration

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Mechanical properties of cells and factor which can change properties have been studied in many previous papers. The extracellular matrix (ECM) has important roles in regulating the development, function and homeostasis of all eukaryotic cells. 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.

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Structural and Dynamic Features of Cold Shock Protein from *Colwellia psychrerythraea*, studied by NMR spectroscopy

이영준 김양미[*]

건국대학교 생명공학과

When temperature drops below the growth temperature, cold-shock proteins (Csps) are expressed. Cold-shock proteins can bind to single-stranded nucleic acids, and this ability allows them to act as RNA chaperones. *Colwellia psychrerythraea* is a Gram-negative psychrophile. The bacteria can survive even in freezing temperature of polar regions. Although cold-shock proteins from various organisms have dramatic differences in their meting temperatures, their amino acid sequences and three-dimensional structures share high similarity. Here, we investigated the structure and dynamics of *C. psychrerythraea* Csp (*Cp*-Csp). *Cp*-Csp contains five β-strands forming barrel structure with hydrophobic core. Psychrophilic *Cp*-Csp defolds at lower temperature(37℃) than its mesophilic and thermophilic homologues do. By analysing 3D structure and the backbone dynamics results, it revealed that *Cp*-Csp has higher structural flexibility and less hydrophobic packing compared to psychrotrophic *L. monocytogenes* Csp and thermophilic *T. aquaticus* Csp. These features, as well as the number of salt bridges, are seems to be key reasons of low thermostability of *Cp*-Csp. This implies that the large conformational flexibility makes the protein to accommodate nucleic acids more easily at extremely low temperature, which is important factor for RNA chaperone function and the cold adaptation of *C. psychrerythraea*.

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3D bioprinting of microporous cell-laden tissue constructs

최기호 김기훈 김민영[1] 신관우[2,*]

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The advancement of tissue and organ engineering lead to bioprinting tissue constructs with cells and cell-laden materials. Bioprinting is an attractive alternative for acellular 3D printing of tissues since cells and cell-laden materials can be precisely positioned to physiologically mimic human tissues. Despite the rapid progress in bioprinting methods, fabrication of cell-laden tissues with microvascular structure and micropores still remained a challenge. Here, we report a method for bioprinting of cell-laden tissue constructs with microvascular structures and micropores. Sucrose is added to increase the viscosity and the printability of the bioink, as well as to create micropores which function as microvasculature. Micropores were fabricated in bioprinted constructs by leaching sucrose crystals after the bioprinting process. These microvascular structures and micropores could improve the fluid flow between cells and the surrounding tissue thereby promoting the cell viability. We studied the effect of micropores on cell viability and diffusion profile in microporous tissue constructs.

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

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서강대학교 화학과 [1]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. Hair was paraffin-embedded and microtome was used to get the cross-section. In each pH, IR spectrums and cross-section images are obtained with FT-IR microspectroscopy and surface images with SEM. Since a hair fiber can be divided into outer layer(cuticle) and inner part(cortex), comparisons between these two parts are also made in each part. 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 conditions will be presented.

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Biochemical characterization of acinetobactin, a major siderophore of *Acinetobacter baumannii*, and preparation of its analogues with improved chemical stability

김학중* 이민욱 송운영

고려대학교 화학과

Since the iron is involved in many functional metabolic processes, its acquisition is essential to maintain the biological processes. However, the human body, one of the habitats of many bacteria, is highly iron-deficient. Therefore, bacteria have developed dedicated iron acquisition system based on the secretion and uptake cycle of small molecules called "siderophores", effective iron chelators. The siderophore-based metabolic mechanism is particularly essential for the survival of the infectious pathogens such as Acinetobacter baumannii. A. baumannii, a Gram-negative bacterium, has recently emerged as one of the most threatening pathogens particularly in the nosocomial settings due to its rapid acquisition of the multidrug resistance. It has been shown that it produce and utilize acinetobactin, fimsbactins, and baumannoferrins as siderophores. Acinetobactin is the major siderophore of A. baumannii, structurally featured by three potential Fe(III) binding moieties; catechol, hydroxamate, and imidazole groups. Previous studies have revealed that the originally reported structure of acinetobactin possessing the oxazoline at its core can be spontaneously rearranged to its isoxazolidinone derivative. Our laboratory have been interested in developing a novel strategy to effectively combat against A. baumannii. In that direction, the employment of "Trojan horse strategy" based on the attachment of antibiotics to acinetobactin has been considered, in which the latter serves as a drug delivery vehicle. For that matter, it is critical to know which of the two structures is the actual siderophore for A. baumannii. To gain some insights into this question, we have prepared acinetobactin as well as systematically designed analogues and characterized their Fe(III) binding and cellular delivery functions. This investigation not only led to the clarification of the physiologically relevant acinetobactin structure, but also revealed several key structural elements for its functionality as a siderophore. Namely, the acinetobactin form possessing the oxazoline core was confirmed to be the physiologically relevant structure. Currently, various structural modifications on this structure are being made to improved its chemical stability as well as the capability to intracellularly delivery the conjugated antibiotics into A. baumannii.

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Assessment of Radiation Exposure and Time Lapse by 2D NMR-based Metabolite Profiling: ^{13}C-Pyruvate Labeling of Metabolites in Human Umbilical Vein Endothelial Cells

채영기

세종대학교 화학과

We employed the endothelial cell model system as a first step toward establishing a method to assess the influence of ionizing radiation by using a combination of common and abundant metabolites. We applied X-ray irradiation amounts of 0, 1, and 5 Gy to the cells that were harvested 12, 24, or 48 h later, and profiled metabolites by 2D NMR spectroscopy to sort out candidate molecules that could be used to distinguish the samples under different irradiation conditions. We traced metabolites stemming from the input ^{13}C-pyruvate, identified 14 of them from the cell extracts, and applied statistical analysis. According to the statistical analysis, lactate and alanine were accumulated with time lapse after irradiation, indicating that the input pyruvate was metabolized to provide a reduction power or a building block. It was interesting to observe that the lactate was accumulated more with increasing irradiation dose while the alanine showed an opposite trend. We hope that this work can form a base for treating radiation-poisoned patients in the future.

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Synthesis of TLR7 Agonists Conjugated Iron Oxide Nanoparticles to Elicit Robust Cytotoxic T Cell Responses via DC Activation

홍성유* 김우겸[1]

UNIST 나노생명화학공학부 [1]UNIST 화학공학과

Recognitionis of pathogen-associated molecular patterns (PAMPs) is the first steps in immune therapy. Especially, Toll-like receptors (TLRs) in dendritic cell (DC) are representative pattern recognition receptors, which is critical for coordinating innate and adaptive immune responses. Imidazoquinolines, known as artificial compounds commerically available as TLR7 agonists, were attacked in aspect of efficiency because of their small size and short half-life in the bloodstream. Here, we synthesized covalent incorporation of imidazoquinoline moieties onto the surface of iron oxide nanoparticles to enhance their chemical stability, cellular uptake efficiency, and adjuvanticity. We utilized copper-catalyzed click reaction (CuAAC) to make novel conjugation between adjuvant and nanoparticles and these synthetic adjuvant-nanocomplexes showed powerful DC activation with lower nanomolar doses. Furthermore we checked unusually strong cytotoxic T lymphocyte responses, by the addition of ovalbumin, because conjugation to macromolecules could induce multivalency effect and efficient transport to endosomal TLR7.

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Aptamosomes targeting both MCF-7 Breast Cancer Cells and Breast Cancer Stem Cells as Drug Delivery System

김동민 김동은*

건국대학교 생명공학과

Recent studies had demonstrated that metformin and aspirin (sodium salicylate) has a remarkable potential for anti-cancer effect by inhibiting AMPK-mTOR signaling pathways. Previously, we have developed an aptamer-conjugated liposomes, namely ‘aptamosomes’, for facile anticancer drug delivery system. In this study, we attempted to prepare for the aptamosome that can co-encapsulate metformin and sodium salicylate to target both 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) specific to cancer cell surface and cancer stem cell surface, respectively. The aptamer-conjugated liposome was prepared by fusing the aptamer-conjugated micelle to plain liposome. The MUC1-aptamosomes showed a specific binding to MCF7 breast cancer cells with fluorescence staining. We observed the cytotoxicity of dual-drug-encapsulating MUC1-aptamosomes to MCF7 cells, which is superior to the aptamosome encapsulated with single drug. We also demonstrated that dual-drug-encapsulating liposomes are significantly more cytotoxic than dual-drug treatment without delivery system. We suggest that the encapsulation of drugs with aptamer-conjugated liposomes can be a useful drug delivery system for treatment of breast cancer by targeting both breast cancer cells and its stem cells.

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Fluorometric Detection of Influenza Virus RNA by RT-PCR Combined with Rolling Circle Amplification-responsive G-Quadruplex

서지나 김동은*

건국대학교 생명공학과

We developed a label-free fluorometric detection system based on double amplification of target nucleic acid by rolling circle amplification-responsive G-quadruplex (GQ-RCA) for sensitive detection of influenza virus RNA. To detect viral RNA with high sensitivity and selectivity, double amplification system was employed through reverse transcription PCR (RT-PCR) coupled in tandem with GQ-RCA. Single-stranded amplified viral DNA (ssDNA) was generated by RT-PCR of samples containing influenza virus RNA. The phosphate-primed DNA strand in amplicon DNA was subsequently degraded by lambda exonuclease. Viral ssDNA formed a ternary RCA initiation complex by annealing to both a partial hairpin primer and a dumbbell padlock DNA template. A long stretch of ssDNA containing repeated copies of the G-quadruplex sequence was generated by RCA at room temperature. Sensitive detection of amplified target nucleic acid was then accomp1lished by monitoring fluorogenic interactions between Thioflavin T (ThT) and RCA-responsive G-quadruplex. Differences in fluorescence intensity between target and non-target viral RNA were evident under UV illumination. Selective fluorescence staining of RCA-responsive G-quadruplex enabled influenza virus RNA detection at concentrations as low as 4.9 aM with a linear detection range between 450 aM to 450 fM. The RT-PCR-coupled GQ-RCA system for influenza virus genome detection exhibited very high sensitivity and allowed convenient multiplexed virus detection within 2.5 h. Thus, a combination of RT-PCR-coupled GQ-RCA and ThT fluorescence staining can be a sensitive and accurate method for detecting RNA molecules of influenza viruses as well as those of other viruses.

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Ferritin Nanocage and Functional Peptides Binding to α-Enolase Relieve Synovial Inflammation in Rheumatoid Arthritis

김가현 정상전*

동국대학교 화학과

Rheumatoid arthritis (RA) is one of the most predominant autoimmune diseases, and antigen-presenting cell (Monocyte and macrophage) and autoantibodies are known to be the main causes thereof. Most recent studies show 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 regulate inflammation by binding to ENO1, but, their proteolytic degradation hinders 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 increase the biological half-life and improve the binding affinity. Ferritin, a protein nanocage composed of 24 identical protein subunits was used to form 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.

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ScFv-Ferritin as an Advanced Targeted Delivery Platform

박선희 정상전*

동국대학교 화학과

Nanoparticles are increasingly used as labels for analytical purposes and therapy. In general, nanoparticles need to be functionalized with single chain variable fragment (scFv). Protein nanocage can self-assembled spherical structure. Small subunits make cluster and they can assembled and disassembled in unique environment. The particles are based on the globular protein shell of human ferritin light chain (HFL). HFL is a self assemble protein. HFL is composed of 24 subunits, which are self-assembled to form a cage-like nanostructure with external diameter of 8 nm. Single chain variable fragments (scFvs) have potential advantages over whole antibodies, scFvs are one-fifth the size of whole antibodies, they retain full antigen binding capacity. It is smaller than IgG but it can binding with antigen and easily make with E.coli system. However its biological half-life is too short and binding affinity is week. This problem is solved with fusion between the nanocage subunit and scFv. Recombinant proteins are formed cluster. So, its biological half-life and binding affinity become better than monomeric scFv.In this study, we developed the therapeutic potential and safety profiles of high affinity protein nanocage (scFv-Ferritin) targeted HER2 antigen which are identified using a scFv variant of Trastuzumab and modified human ferritin light chain. We show that protein nanocage demonstrate high binding affinity and specificity to HER2 antigen. Moreover the binding affinity of the protein nanocage was determined to be higher than monomeric scFv and whole Trastuzumab. The fluorescence labeled protein nanocage successfully functioned in xenograft models of breast cancer (HER2-overexpressing breast cancer cells). In order to increase the toxicity of nanocage, it was conjugated by maleimide doxorubicin. Doxo conjugated nanocage' s toxicity is measured by MTT assay. It works better than just doxorubicin. Due to its molecular level engineering capability and increased binding avidity, ScFv-ferritin is expected to be a novel delivery platform for theragnosis.

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Effect of Ginkgolic Acid on Adipogenesis in Mature 3T3L1 Adipocytes And Antidiabetic Activity

이지희 정상전*

동국대학교 화학과

Diabetes has become an epidemic in many countries and is associated with many metabolic complications, including obesity, insulin resistance, hyperlipidemia, heart disease, and osteoarthritis. Particularly, Type 2 diabetes mellitus (T2DM) is the most common form of diabetes, occupying 90% of the diabetic population. The insulin resistance in T2DM is due to decreased glucose uptake level and attenuated stimulation of muscle glycogen synthesis. glucose metabolism in adipose tissue play a critical role in glucose homeostasis through transporting glucose into the cells when blood glucose level is high. Therefore, various compounds have been explored for their anti-diabetes effects in adipocytes recently. Here, we demonstrated the effect of ginkgolic acid (GA) in insulin signaling pathway. we report that GA help to maintain insulin sensitivity in 3T3-L1 adipocytes through the AMP-activated protein kinase (AMPK) pathway. AMPK directly modulates fatty acid synthesis and oxidation by altering the activation of enzymes and proteins involved in fat metabolism. Taken together, these results indicate that GA exerts anti-diabetes effects by activating the AMPK signal pathway and that GA might be a potential therapeutic candidate for the prevention or treatment of Type 2 diabetes.

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Development of a fluorescence based system for detecting and inhibitor screening of Amyloid-β aggregation

양승현 정상전*

동국대학교 화학과

Alzheimer's disease (AD) is caused by aggregates of amyloid-β peptide in the brain. The formation of amyloid fibril is associated with the interactions of high concentration of metal ion and extracellular amyloid-β peptide deposits in the brain. The rate of amyloid-β aggregation is promoted by various factors, particularly high concentration of zinc ion (Zn2+) is coordinated with His13, His14 and Asp1 site of the amyloid-β peptide. [1] Based on this mechanism, the detection of amyloid-β peptide aggregation and development of the inhibitor is primary object of diagnostic and therapeutic strategies against AD. The current systems to detect amyloid-β peptide aggregation and screening inhibitor are Western blot (WB), ELISA, TEM, immunoprecipitation (IP).[2, 3] However, these common systems are complicated, time-consuming and costly. To overcome this drawback, a rapid and robust detection method is designed, based on the direct fluorescence detection. Our strategies are fluorescence detection of increased or decreased fluorescence intensity by changing amyloid-β folding formation correlated with the concentration of zinc ions. This system was proved by inhibitor compound L2-b that is known to prevent amyloid-β aggregation in the cell. [4] Applying this strategy, we are testing several natural compounds that is expected to inhibit aggregation and screening inhibitor compound such as small molecule or peptide drug. In addition, we revealed evidence of a amyloid-β peptide conformational change mechanism.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **BIO.P-327**
발표분야: 생명화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Clustering effect of Interleukin 1 receptor antagonist on the ferritin light chain

우수련 정상전[1,*]

동국대학교 화학과 / 화학생물학실험실 [1]동국대학교 화학과

To overcome Rheumatoid arthritis which is autoimmune disorder due to overexpressed inflammation mediated cytokines, therapeutic fusion protein is newly discovered. The therapeutic fusion protein showing clustering effect is made with the two main proteins. ‘ferritin’ for the self assembling nanocarrier construct and ‘interleukin 1 receptor antagonist’ for the therapeutic function. Ferritin is iron carrier protein forming self assembled globular protein complex consisting of 24 subunits. and another therapeutic part is the recombinant form of the naturally occurring IL1Ra(Interleukin 1 receptor antagonist) which prevents Interleukin 1 receptor binding of either IL-1a or IL-1b ,signaling acute phase inflammation abnormally. We linked Ferritin light chain gene and interleukin 1 receptor gene, then soluble expressed in the Escherichia coli system. constructed 24mer self assembled ball like nanocarrier was coated with therapeutic proteins. Thanks to its larger size, this fusion protein can stay longer than just therapeutic protein itself and through clustering effect it can more strongly and specifically bind to the target than conventional targeting therapy. Globular self assemble structure formation was confirmed with TEM image. This fusion protein shows higher functionality at targeting. further, carrier shape can embed some drug or detection molecule. It has vast possibilities to be applied in many scientific field.Reference.1. Dinarello, C. A., A. Simon and J. W. van der Meer (2012). "Treating inflammation by blocking interleukin-1 in a broad spectrum of diseases." Nat Rev Drug Discov 11(8): 633-652.2. Kang, H. J., Y. J. Kang, Y. M. Lee, H. H. Shin, S. J. Chung and S. Kang (2012). "Developing an antibody-binding protein cage as a molecular recognition drug modular nanoplatform." Biomaterials 33(21): 5423-5430.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-195**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

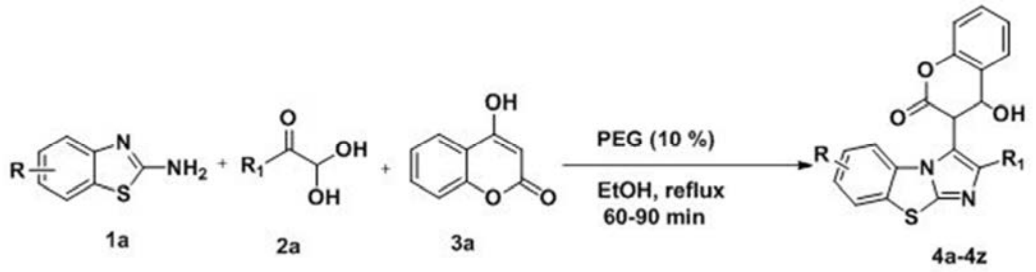
Polythene glycol (PEG) as a green solvent system for the synthesis of novel Benzo[d]imidazo[2,1-b]thiazol-3-yl)-2H-chromen-2-one under catalyst free conditions

Sandip Gangadhar Balwe 정연태*

부경대학교 융합디스플레이공학과

A cost-effective and eco-friendly, straightforward synthesis of highly diversified a novel class of benzo[d]imidazo[2,1-b]thiazol-3-yl)-2H-chromen-2-one scaffold is successfully achieved via one-pot three-component cascade reaction utilizing 2-aminobenzothioazole, arylglyoxal monohydrate and 4-hydroxycoumarin in ethanol–PEG-600. Tedious work-up procedures, column purifications are avoided because of the direct precipitation of products from the reaction solution.

Scheme



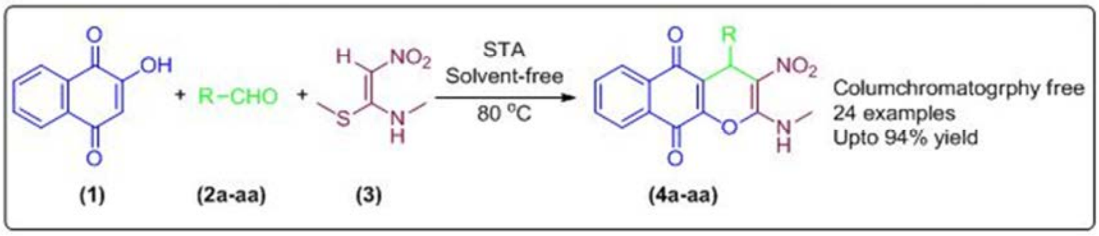
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-196**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Silica-supported tungstic acid (STA) as a highly efficient and reusable heterogeneous catalyst for the synthesis of 4H-pyranonaphthoquinones under neat conditions

KRISHNAMMA GARI SURESH KUMAR 정연태*

부경대학교 융합디스플레이공학과

An efficient, simple and green one-pot domino protocol for the synthesis of benzo[g]chromene-5,10-diones has been synthesized by multi-component condensation of 2-hydroxy-1,4-naphthoquinone with aldehydes and (E)-N-methyl-1-(methylthio)-2-nitroethenamine in the presence of silica-supported tungstic acid (STA), affording excellent yields under neat conditions. This transformation presumably occurs through a sequential aldol reaction, Michael addition, imine-enamine tautomerism-intramolecular, O-cyclization, elimination sequence of reactions. The significant features of this reaction include short reaction time, high yields, eco-friendly method, and no need column chromatography technique. Furthermore the catalyst can be recycled up to four times without losing its catalytic activity.



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-197**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

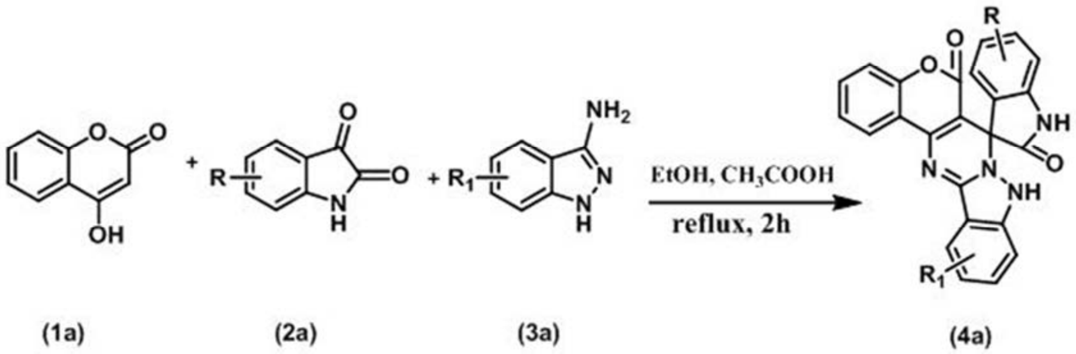
A novel three-component method for the synthesis of spiro-[chromeno[4',3':4,5]pyrimido[1,2-b]indazole-7,3'-indoline]-2',6(9 H)-dione

Amol Maruti Jadhav 정연태*

부경대학교 융합디스플레이공학과

A novel and efficient one-pot synthesis of spiro[chromeno[4',3':4,5] pyrimido[1,2-b]indazole-7,3'-indoline]-2',6(9 H)-dione derivatives via three-component reaction of 4-hydroxy-2H-chromen-2-one, isatin, and 1H-indazole-3-amine, in the presence of acetic acid in EtOH. The advantages of this method include high efficiency, mild reaction conditions, convenient operation, and environmentally benign conditions.

Scheme



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-198**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of carotenoid using chain extension unit

김다혜 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carotenoids 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 food, health care products, etc. 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(BT) 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 BT sulfone containing an acetal group was prepared as an building block for the chain extension of apocarotenoids. The Julia-Kocienski olefination of the BT 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 BT sulfone.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-199**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A study on the synthesis of fully conjugated units for carotenoid

강세인 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Carotenoids are important natural products Which have medical, biological effect. We studied the synthesis of the natural carotenes using sulfone-mediated coupling reaction, protection of alcohol and double elimination. 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 natural carotenoid and electronic conductivity of carotenoids.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-200**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A study of synthetic method for Unnatural carotene wire

임보람 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Unnatural carotenoids containing various phenyl substituents compared with Natural carotenois in terms of stability as well as electronic characteristics. We have perfectly demonstrated the efficient synthesis of natural carotenoids, which can be further extended to the synthesis of unnatural carotenoid wires. The unnatural carotenoids can be assembled by the coupling and double elimination reactin between haloallylic sulfone with dialdehyde unit. allylic sulfone moiety attaching aromatic phenyl groups containing para-substituents X(OMe,Me,H and Cl) can be prepared from acetophenone derivatives. Therefore, We were able to measure electrical conductivity for various carotenoid wires.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-201**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Measurement of Conductance of the Carotenoid 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.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-202**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of unnatural carotenoids

유혜빈 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

Unnatural carotenoids containing various Phenyl substituents exhibit an advantage in terms of stability and electronic characteristics, compared with the natural carotenoids. Chain extension of triene-dialdehyde unit using Julia-Kocienski olefination efficiently provided an extended dialdehyde unit. The Julia-Kocienski olefination of the Phenyl-substituted-C5 -BT(benzothiazole)-sulfone with C10 2,7-diphenyl-2,4,6-octatrienedial efficiently produced tetra-Phenyl-substitued-dial. Carotenoid molecular wires can be assembled by the Wittig reaction between tetra-Phenyl-substituted-dial with 4-thiomethylbenzyl phosphonium bromide.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-203**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

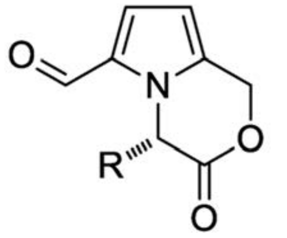
Practical Synthetic methods of Pyrrolo Lactone compound

인익준 구상호[1,*]

명지대학교 에너지융합공학과 [1]명지대학교 화학과

The compounds 1a and 1b are the key components of traditional folk medicine extracted from Celastrus orbiculatus and Capparis spinosa respectively. The Maillard reaction between amino acid and sugar produces various volatile products. The Malilard reaction produces very little amount of pyrrole form [1]. We developed a mild Mailard variant, which reacted sugar and amino acid in oxalic acid and DMSO at 65~90°C to give 30~40% yield of pyrrolo lacton [1]. This reaction can make various amino acids and sugars easily and practically for [1] form. Diversely R-substituted pyrrolo lacton [1] can be obtained depending on the form of amino acid. It is expected that this pyrrolo lactone compound can possibly be the next generation of analgesic drugs, human-friendly seasonings and functional materials.

1



a : R = Methyl
b : R = Benzyl

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-204**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A study on the synthetic method for nano molecular wire

김민수 구상호[1,*]

명지대학교 에너지융학공학과 [1]명지대학교 화학과

Nanoscience and engineering requires for the smaller, faster, and flexible substitutes for the conventional metallic wire. Organic molecular wires with variable conductance is one of the urgent goals in molecular electronics. Organic molecules containing terminal thiol group can be used in electronic conductance using Atomic Force Microscopy(c-AFM). Existence of extensive π-conjugation offer high electronic conductance because of the delocalized π-electron system. Delocalized π-electron in carotenoids are good for electronic conductance. 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 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-205**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on the Mn(Ⅲ)-initiated radical oxidation and the application on the synthesis of natural products

JIANG XIA 구상호[1,*]

명지대학교 에너지융합공학과 [1]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 using Mn(Ⅲ)/Co(Ⅱ) catalytic oxidative deacetylation. Further work on extending this catalytic oxidative reaction to the synthesis of some natural products is ongoing.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-206**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Axially chiral biaryl dials as a chiral shift reagent

정은정 이기성 이성언 한호규*

고려대학교 화학과

Abstract Body: Axially chiral biaryl dials were synthesized and studied for their use as a chiral shift reagent (CSR). The various amino esters were derivatized with the two enantiomers of these dials and the chemical shift differences between thus obtained diastereomeric imines were investigated.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

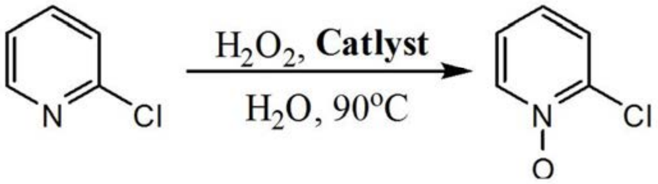
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-207**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Catalyst for Oxidation of Pyridine to Pyridine N-oxide using Hydrogenperoxide

이상희* 김동희 김세미

군산대학교 화학과

2-Halopyridine N-oxides, especially 2-chloropyridine N-oxide, are important intermediate products for example in the preparation of pyrithiene, especially zinc pyrithione, which are effective as bactericides and fungicides. Because of the electron-withdrawing properties of the halogens, 2-halopyridines can be oxidised with greater difficulty than other pyridine derivatives. Here, effective and reusable nonmetallic catalyst for oxidation of 2-haloptridine to N-oxide using aqueous hydrogen peroxide, will be described.


N
Cl
H_2O_2, **Catlyst**
H_2O, 90°C
N
Cl
O

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-208**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Novel Synthesis of 5-phenyl-2-heteroarylcarbothioamides from heteroarylcarboxylic acids

이희주 김한나 이재인*

덕성여자대학교 화학과

Thioamides are an important compounds class due to their diverse biological activities and especially [5-(3,4-dichlorophenyl)furan-2-yl](piperidin-1-yl)methanethione (DFPM) downregulates abscisic acid (ABA)-dependent gene expression and inhibits ABA signal induction. A synthetic route of 5-phenyl-2-heteroarylcarbothioamides is described. The diazotization of 2-furoic acid with benzenediazonium salts afforded 5-phenyl-2-furoic acids which were treated with di-2-pyridyl carbonate(2-DPC) and subsequent addition of amines to give 5-phenyl-2-furancarboamides in one-pot. 5-Phenyl-2-heteroarylcarboamides were also prepared by the coupling of 5-bromo-2-heteroarylcarboamides with sodium tetraphenylborates in the presence of catalytic palladium(Ⅱ) chloride. The thionation of 5-phenyl-2-heteroarylcarboamides using Lawesson reagent afforded 5-phenyl-2-heteroarylcarbothioamides in high yields.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-209**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A study on chemical probes targeting protein aggregates associated with neurodegenerative diseases

이현승 민선준[1,*]

한양대학교 응용화학과 [1] 한양대학교 과학기술대학/응용화학과

Alzheimer’s disease is characterized by aggregation of two hallmarks, tau and amyloid beta. Recent studies, however, showed that soluble aggregated Tau species, especially hyperphosphorylated Tau oligomers, which are formed at early stage of AD prior to the formation of Neurofibrillary tangles (NFT), disrupted neural system integration. Unfortunately, little is known about Tau aggregates, and few Tau targeted imaging probe has been reported.

Development of noninvasive bioimaging probes for trapping tau fibrils is highly desirable for early diagnosis of AD. The diverse optical imaging techniques using visible, ultraviolet, and infrared light have been developed. Among them, fluorescence imaging in the near- infrared (NIR) spectral region has been attracted for noninvasive *in vivo* imaging. Biomolecules have low absorption and autofluorescence in the NIR region, which allows the NIR imaging technique to detect target molecules in an optimal penetration depth with high sensitivity. Therefore, there has been growing interest in the NIR fluorescence imaging of tau fibrils for noninvasive diagnosis.

Herein, the synthesis and *in vitro* evaluation of new indane derivatives as NIR chemical probes for detection of Tau aggregates is described. A series of indanes having substituted styrenes with push-pull structures were synthesized via Pd catalyzed coupling reactions. The fluorescence properties of these compounds were tested with or without tau fibrils in order to confirm their interaction with tau aggregates. Our preliminary result and discussion of this study is presented in this poster.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-210**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The conjugated polymers based on 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole(TTI) and isoindigo for organic photovoltaics

윤준태 서홍석*

부산대학교 화학과

Conjugated polymers using 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole (TTI) and isoindigo (ID) were fabricated for high performance. The alternating copolymer and random copolymers including TTI and ID units were designed. The UV-vis absorption spectra of the random copolymers displayed greatly red shifted at maximum peaks and a more broad full width at the half maximum (fwhm) with rasing rate of ID unit. Conjugated polymers show deeper highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels with increased percentage of ID as electron accepting groups. When compared the alternating copolymer PTTIID with the random copolymer PTTIID-7, random copolymer PTTIID-7 showed higher J_{SC} and FF values owing to the better morphology and proper hole mobility, making higher PCE value. The device composed of PTTIID-7 and PCBM (1:2) with chloronaphthalene (CN) additive showed a V_{OC} of 0.63 V, a J_{SC} of 12.3 mA/cm^2, and a fill factor (FF) of 0.52, giving a power conversion efficiency (PCE) of 4.03%.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-211**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Strategies for improving high efficiency by using 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole and fluorinated benzothiadiazole for organic solar cells

윤준태 서홍석[*]

부산대학교 화학과

Polymer solar cells (PSCs) is the most powerful alternative energy source because of their strong points such as low cost, large area, ultra-weight and solution processing. To grow the power conversion efficiency(PCE) up, we designed and successfully synthesized polymers, fluorinated dithienylbenzothiadiazole (DTBT) as an electron accepting group and 6-(2-thienyl)-4*H*-thieno[3,2-*b*]indole as an electron donating group. One of the strategies for high efficiency in organic solar cells is that fluorine atom is introduced in conjugated polymer because of the strong electron-withdrawing ability of fluorine, the synthesized polymers with fluorine atom indicated deep high molecular orbital (HOMO) energy levels. The device using the PTTIF1:$PC_{71}BM$ (1:1w/w) blend without additive showed power conversion efficiency (PCE) of 3.71% and the device using the PTTIF2:$PC_{71}BM$ (1:1w/w) blend with chloro-naphthalene (CN) additive showed PCE of 4.36%.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-212**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis conjugated polymers composed of pyrimidine derivatives and applications in organic solar cells

윤준태 서홍석*

부산대학교 화학과

Organic solar cells have recently attracted attention because of their advanced properties including low expense, light-weight, mechanical flexibility, simple processability and large-scale production. We synthesized conjugated polymers composed of PTTICN, PTTICNR and PTTIFR based on TTI, 2-fluoropyrimidine and 2-pyriminecarbonitrile. The optical band gaps of PTTICN, PTTICNR and PTTIFR were about 2.0 eV. The synthesized polymers (PTTICN, PTTICNR and PTTIFR) showed deep HOMO energy levels between -5.26 and -5.34 eV. The device based on PTTICN and $PC_{71}BM$ (1:4) with DIO showed a V_{OC} of 0.82 V, a J_{SC} of 6.38 mA/cm^2, and a fill factor (*FF*) of 0.54, having a power conversion efficiency(PCE) of 2.81%. The device based on PTTICNR and $PC_{71}BM$ (1:4) with DIO exhibited a V_{OC} of 0.81 V, a J_{SC} of 6.38 mA/cm^2, and a *FF* of 0.43, having a power conversion efficiency(PCE) of 2.22%. The device based on PTTIF and $PC_{71}BM$ (1:4) with DIO exhibited a V_{OC} of 0.64 V, a J_{SC} of 7.38 mA/cm^2, and a *FF* of 0.55, having a power conversion efficiency(PCE) of 2.61%.

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발표분야: 유기화학
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Novel donor-acceptor conjugated polymers based on indenoindene for organic photovoltanics(OPVs)

윤준태 서홍석*

부산대학교 화학과

The novel conjugated polymers including dihydroindeno[2,1-*a*]indene moiety (ININE), with greatly planar electron-donating ability, was designed. The donor-acceptor conjugated polymers, P1 and P2 have a electron accepting unit of *N*-alkyl-2,2′-bithiophene-3,3′-dicarboximide (BTI) and electron donating unit of ININE. These polymers were composed by coupling electron donating and accepting units with Stille polymerization, using Pd(0) catalyst. Two synthesized polymers showed deep energy levels of HOMO between -5.76 and -5.59 eV and proper energy levels of LUMO between -3.65 and -3.55 eV. The PCE of P2 was the higher than the PCE of P1. The device comprising P2 and $PC_{71}BM$ (1:2) with DPE showed a V_{OC} of 0.80 V, a J_{SC} of 1.59 mA/cm^2, and a fill factor (*FF*) of 0.39, giving a power conversion efficiency of 0.49%.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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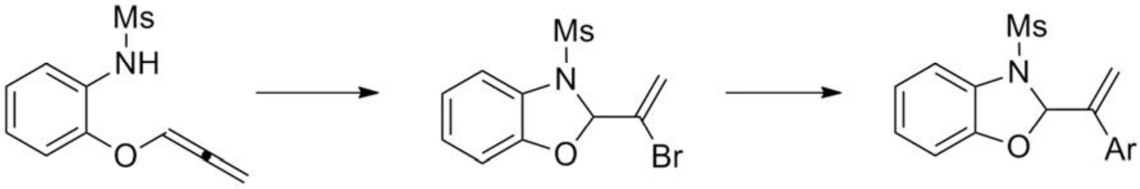
장소: 일산 KINTEX
발표코드: **ORGN.P-214**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthetic study of benzoxazole derivatives by palladium-catalysed cyclization of allenyl ether

최지혜 김건철*

충남대학교 화학과

Allenes, which are more reactive than other unsaturated groups, are extremely versatile functional groups in organic synthesis. In this study, benzoxazole derivatives have been synthesized by intramolecular carbo- and hydroamination of allenyl ether by using palladium catalyst. Moreover, Haloamination followed by Suzuki coupling, Heck, and Sonogashira reactions were attempted to synthesize various derivatives.



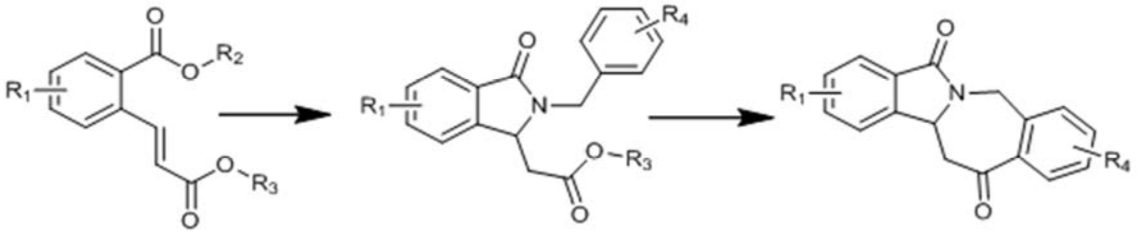
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-215**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Study on the synthesis of isoindolobenzazepine alkaloids

이건중 김건철*

충남대학교 화학과

The interest in the development of methods for the synthesis of tetracyclic structures in which an isoindole fragment is annulated with quinoline, or benzazepine fragments is due to the wide spectrum of physiological activity and the widespread occurrence of such structures in nature. Among them the structure of isoindolobenzazepine is tetracyclic compounds including both isoindolinone and benzazepine fragments. In this study a new attempt has been designed to form the skeleton by intramolecular Michael addition and Friedel-Craft type reaction



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발표코드: **ORGN.P-216**
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발표종류: 포스터, 발표일시: 목 11:00~12:30

Total synthesis of resorcylic lactones: Aternariol using BBr3-promoted intramolecular cyclization without formation of side products

권소현 김태현[1,*]

인천대학교 화학과 [1]인천대학교 자연과학대학 화학과

Alternariol, main metabolite of toxin-producing Alternaria fungi, leads to crop losses by fouling of some fruits such as tomatoes, apples despite of low toxicity as compared with others. Therefore, the isolation of alternariol is an important issue for minimization of crop losses and toxicological residual risks. However, only sub-milligram amounts of the Alternariol can be obtained from infected fruits, so artificial synthesis of Alternariol is necessary. Total synthesis of alternariol is already proposed in other studies, but the final synthesis step gave poor yield, together with the generation of side-products. For this reason, we tried to search new high-yielded procedures and conditions, and the new synthesis of alternariol using BBr3-promoted intramolecular cyclization has been developed.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-217**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly sensitive colorimetric chemosensor based on thiourea for fluoride ion detection

유혜림 김태현[1,*]

인천대학교 화학과 [1]인천대학교 자연과학대학 화학과

Anions play an important role in a wide range of chemical and biological processes.Fluoride ion, in particular, has drawn particular interest due to its impact on the environment and health. Thiourea binding sites is widely used as a colorimetric sensor for sensing fluoride ions. Sensors including thiourea can detect fluorine ions selectively.In this study, we synthesized highly sensitive colorimetric sensor containing thiourea unit for fluoride ion detection. Due to the specific structure of the receptor containing multiple amine groups, our sensor molecule is expected to detect fluoride ions effectively through the hydrogen bonding. The synthesis, characterization and and properties of the newly-developed chemosensor will be detailed.

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장소: 일산 KINTEX
발표코드: **ORGN.P-218**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A Practical Synthetic Method for the Unsymmetrical Ureas from Trichloroethyl Carbamates Using DBU

김희권

전북대학교 의학전문대학원/핵의학교실

Urea is a common basic structure found in many natural compounds and biologically active compounds. In additions, various research areas such as supramolecular polymers and drug discovery have utilized urea unit. Herein, a facile synthesis of unsymmetrically substituted ureas is presented. By using small amount of 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU), several unsymmetrical ureas was readily prepared from the 2,2,2-trichloroethyl carbamate compounds and many amines. This synthetic method offered preparation of various di-and trisubstituted with good yields. It was also possible to synthesize tetrasubstituted ureas in moderated yields. This study gives a potential approach for efficient and practical synthesis of many unsymmetrical ureas from 2,2,2-trichloroethyl carbamates.

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장소: 일산 KINTEX
발표코드: **ORGN.P-219**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Diversification of pyrrolo[2,3-d]pyrimidine by microwave mediated Cu-catalyzed *N*-arylation coupling reaction

박승영 염을균*

충남대학교 화학과

Arylpyrrolo[2,3-d]pyrimidines have shown wide range of biological activitys, such as anti microbial, inhibition of protein kinases and antagonist effects to receptors, etc. Thermal C-N coupling reaction needs long time and requires harsh conditions to synthesize these derivatives. but microwave reaction has the advantage of reducing time and reducing side effects compared to thermal reaction. In this study, we will discuss about using the microwave unlike thermal reaction then N-arylated pyrrolo[2,3-d]pyimidine and their derivatives are synthesized within a short reaction time and high yield.

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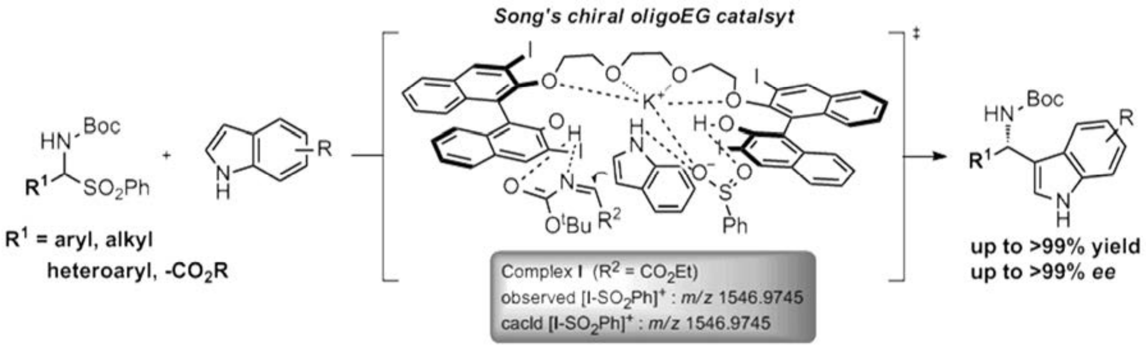
발표코드: **ORGN.P-220**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Cooperative Cation-Binding Catalysis as a Efficient Approach for Enantioselective Friedel-Crafts Reaction of Indoles and Pyrrole

김문종 송충의*

성균관대학교 화학과

We developed a highly enantioselective Friedel-Crafts reaction of indoles, 4,7-dihydroindole and pyrrole with α-amidosulfones as sensitive imine surrogates using a cooperative cation-binding catalyst. In this new catalytic protocol heteroaromatic and aliphatic substrates as well as α-imino ethyl glyoxylate also afforded the desired products with excellent yields and ees. Thus, this method enables the catalytic synthesis of biologically interesting natural products and pharmaceutically relevant chiral Friedel-Crafts indole/pyrrole adducts. Due to the conformational stability of the transition state at high temperature, all the proposed intermediates were identified by the ESI-MS analysis. Furthermore, the key to this successful catalytic activity is the cation-binding catalysis in a densely confined chiral space in situ formed by the incorporation of potassium salt. Like enzymes in a confined space, thus enhancing the reactivity and efficiently transferring the stereochemical information.



일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-221**

발표분야: 유기화학

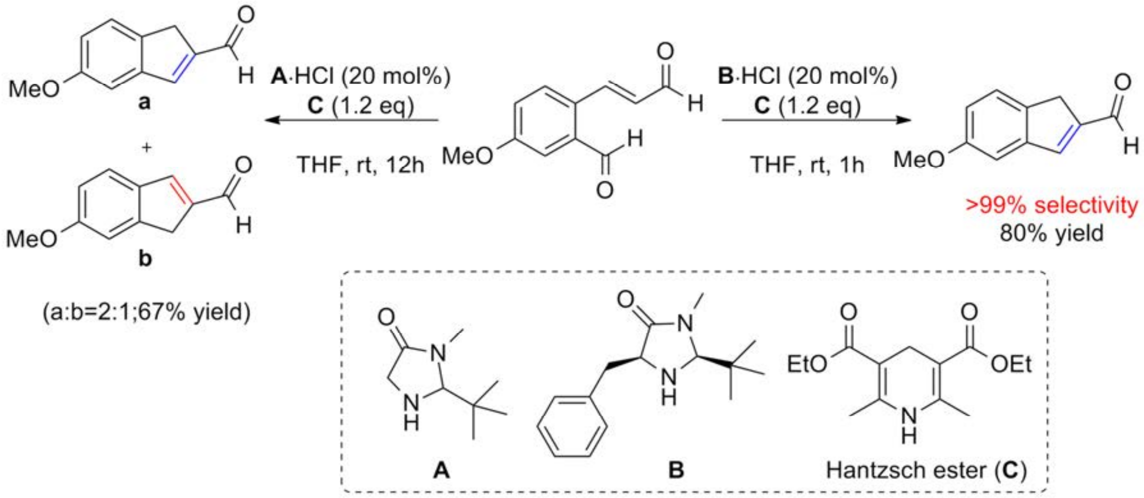
발표종류: 포스터, 발표일시: 목 11:00~12:30

Organocatalytic regiospecific synthesis of 1H-indene-2-carbaldehyde derivatives: suppression of cycloolefin isomerisation by employing sterically demanding catalysts

신훈이 송충의[1,*] 양정운[*]

성균관대학교 에너지과학과 [1]성균관대학교 화학과

Indenes are utilised as building blocks in organic syntheses, and they often appear as the key structural motif in many natural products with interesting biological activities and in functional materials. For these reasons, the construction of an indene ring system has become a hot topic of interest for chemists. To date, a variety of synthetic methods to facilitate the formation of an indene ring have been reported. Although transition-metal catalysis are widely used in the synthesis of a wide range of different substituted indenes, there are still important regioselectivity issues concerning multi-substituted indene derivatives that need to be addressed. Here, we have demonstrated a highly regiospecific fashion for the synthesis of 1H-indene-2-carbaldehyde derivatives through transition-metal-free, cascade reductive cyclisation of ortho-formyl trans-cinnaldehydes with Hantzsch ester in the presence of an aminocatalyst. Especially, cycloolefin isomerisation of the resulting products could be inhibited efficiently by the introduction of a sterically demanding stereo-defined aminocatalyst.


MeO
a
+
MeO
b
(a:b=2:1;67% yield)
A·HCl (20 mol%)
C (1.2 eq)
THF, rt, 12h
MeO
B·HCl (20 mol%)
C (1.2 eq)
THF, rt, 1h
MeO
>99% selectivity
80% yield
A
B
EtO
OEt
Hantzsch ester (C)

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장소: 일산 KINTEX
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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Efficient blue emitting materials based on dibenzochrysene for Organic Light Emitting Diodes

김창민 강지수 조석원 윤승수*

성균관대학교 화학과

In this study, we synthesized six deep blue fluorescent materials (1-6) based on dibenzochrycene moiety for organic light emitting diodes (OLEDs). To investigate their electroluminescent (EL) properties, multilayered OLEDs with the following sequence; indium-tin-oxide (ITO) / 4,4′,4″-Tris[2-naphthyl(phenyl)amino]triphenylamine (2-TNATA) (30 nm) / N,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) (20 nm) / Blue emitting materials (30 nm) / bathophenanthroline (Bphen) (30 nm) / lithium quinolate (Liq) (2 nm) /Al (100 nm) were fabricated using synthesized materials as emitters. All devices exhibited efficient blue emissions.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **ORGN.P-223**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Indenophenanthrene Derivatives for Blue Organic Light-Emitting Diodes

강지수 김창민 조석원 윤승수*

성균관대학교 화학과

Herein, we designed and synthesized four blue emitting materials based on indenophenanthrene derivatives. Light-emitting devices using these materials were fabricated in the following sequence; indium-tin-oxide (ITO) (180 nm) / 4,4′,4″-Tris[2-naphthyl(phenyl)amino] triphenylamine (2-TNATA) (30 nm) / N,N'-diphenyl-N,N'-(2-napthyl)-(1,1'-phenyl)-4,4'-diamine (NPB) (20 nm) / Blue materials (30 nm) / 4,7-diphenyl-1,10-phenanthroline (BPhen) (30 nm) / lithium quinolate (Liq) (2 nm) / Al (100 nm). All devices showed blue emissions efficiently.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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An Efficient Method for the Amide unit from Alloc-Protected Ester Using DABAL-Me_3

김희권

전북대학교 의학전문대학원/핵의학교실

Amide is commonly found in many natural compounds and organic compounds. The synthesis of amides from carboxylic acid derivatives is useful transformation. Moreover, direct formation of amides from the protected ester is attractive in organic chemistry areas. Herein, novel synthetic method for the amide from Alloc-protect ester is described. In the novel synthesis, DABAL-Me_3 was utilized to treat ester derivatives to produce the corresponding amides. Particularly, novel reaction protocols do not require exclusion of air or moisture, and all transformation to amides from Alloc-protected ester achieved in high yield. This study offers a useful approach for synthesis of a variety of amide.

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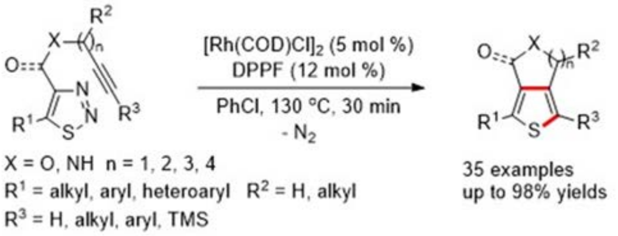
Rhodium-Catalyzed Intramolecular Transannulation Reaction of Alkynyl Thiadiazole Enabled 5,n-Fused Thiophenes

서보람 엄규식 이필호*

강원대학교 화학과

Fused thiophenes have been recognized as very important scaffolds in the field of pharmaceutical and functional materials sciences. For this reason, the development of an efficient synthetic method for functionalized fused thiophenes is highly attractive and poses a significant challenge. However, because some of the previously reported synthetic methods demand a strong base, long reaction times, and vigorous reaction conditions, the development of efficient synthetic approaches to overcome these shortcomings has been continuously required.Herein, we developed a method for the synthesis of a wide range of fused thiophenes, including those fused with lactams, lactones, or cyclic ethers, from a rhodium-catalyzed intramolecular transannulation reaction of alkynyl thiadiazoles. This transannulation reaction provides an efficient platform for the construction of a variety of 5,n-fused thiophenes from readily available starting materials together with the release of molecular nitrogen.This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2011-0018355), 2015H1C1A1035955.



- ✓ ***Modular synthesis of 5,n-fused thiophene***
- ✓ ***Versatile ring size and type***
- ✓ ***Simple operation***
- ✓ ***Short time***

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발표분야: 유기화학
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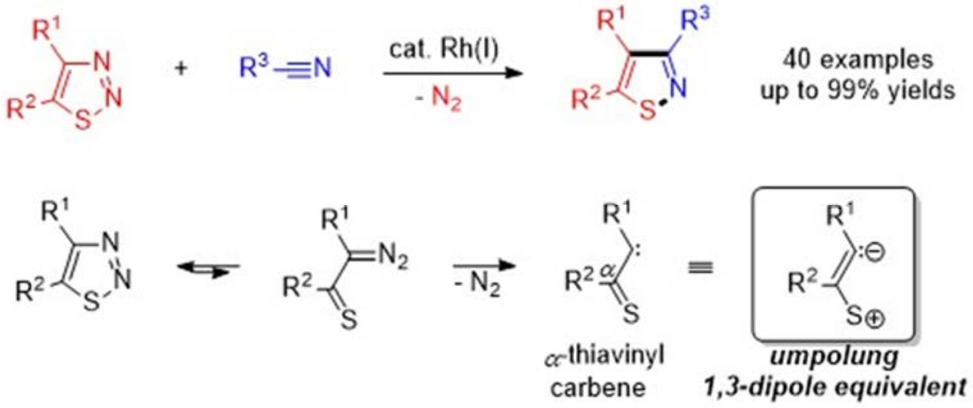
Synthesis of Isothiazole *via* the Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Nitriles

서보람 허남림 이필호*

강원대학교 화학과

Isothiazoles are valuable structural motifs found in many natural products, pharmaceutical compounds, and functional materials. For this reason, streamlined methods for their synthesis from readily available compounds must be developed.Herein, we developed a synthetic method for obtaining a wide variety of isothiazoles by the Rh-catalyzed transannulation of 1,2,3-thiadiazoles with alkyl, aryl, and heteroaryl nitriles, which proceeds *via* an α-thiavinyl Rh-carbenoid intermediate. The results suggest that during its reaction with nitriles, the α-thiavinyl carbene acts as an umpolung 1,3-dipole equivalent, in contrast to its behavior during its reaction with alkynes. The developed method was successfully employed to synthesize pentaoligomeric arylene compounds consisting of three benzene and two isothiazole rings.



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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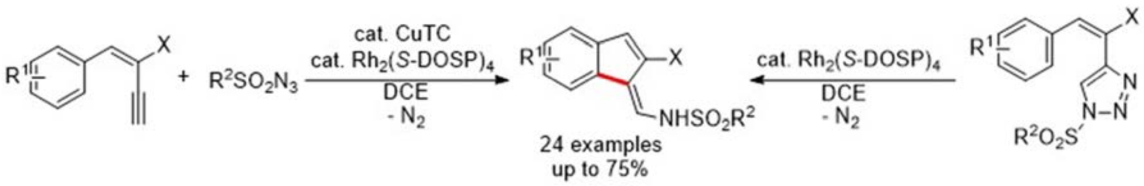
장소: 일산 KINTEX
발표코드: **ORGN.P-227**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Benzofulvenes through Rhodium-Catalyzed Transannulation of Enynyl Triazoles

연의성 변민현 이필호*

강원대학교 화학과

Benzofulvenes are key privileged scaffolds present in natural products, biologically and pharmacologically active molecules, functional materials, and metallocene catalysts. Due to its significance, it is still of considerable interest and necessity to develop efficient synthetic methods for functionalized benzofulvenes. Recently, N-sulfonyl-1,2,3-triazoles, easily obtained from click reactions, have been used for the preparation of a large number of heterocyclic and carbocyclic compounds through Rh-catalyzed denitrogenative cyclization.On the basis of these results, Rh-catalyzed denitrogenative cyclization of (*E*)-ethyl 2-(1-alkyl and arylsulfonyl-1*H*-1,2,3-triazol-4-yl)-3-aryl acrylate generated from (*E*)-ethyl 2-benzylidenebut-3-ynoates and *N*-sulfonyl azides in the presence of a copper catalyst was demonstrated for the synthesis of a wide range of functionalized benzofulvenes. Additionally, we have developed straightforward synthetic procedures for three benzofulvenes through tandem Cu-catalyzed [3 + 2] cycloaddition and Rh-catalyzed denitrogenative cyclization from (*E*)-ethyl 2-benzylidenebut-3-ynoates and *N*-sulfonyl azides in a one-pot.



R^1 = H, 2-Me, 3-Me, 4-Me, 4-MeO, 3,5-$(MeO)_2$, 4-Cl, 3-Br, 4-AcO, 2-F-4-MeO
R^1-C_6H_4 = 2-naphthyl, 2-furyl R^2 = Me, *i*-Pr, 4-Me-C_6H_4, 4-MeO-C_6H_4
X = CO_2Et, CH_2OMe, Ac

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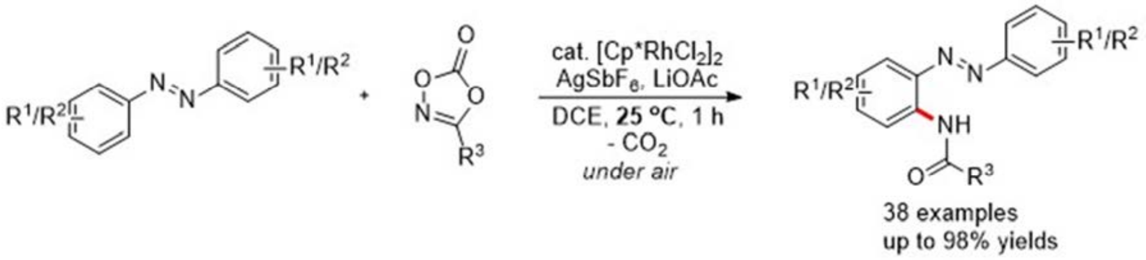
Selective Rh-Catalyzed C-H Amidation of Azobenzenes with Dioxazolones under Mild Conditions

연의성 엄규식 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. Hrerin, 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 National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2011-0018355), 2015H1C1A1035955.



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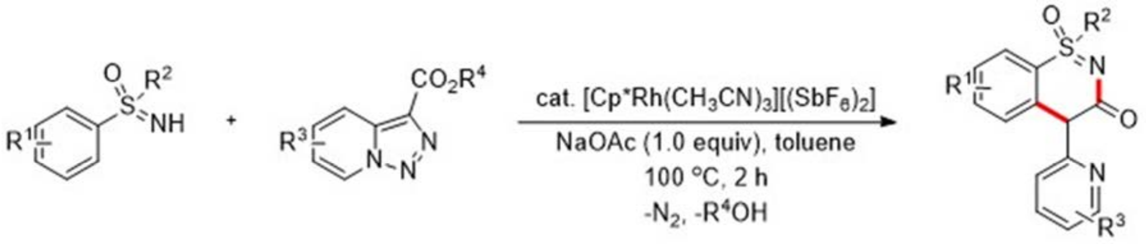
Synthesis of 1,2-Benzothiazines through a Rh-Catalyzed Cascade C-H Activation/Cyclization/Elimination from Sulfoximines and Pyridotriazoles

손정유 고기훈 이필호*

강원대학교 화학과

Sulfoximines are novel privileged scaffolds that have been applied as pharmaceuticals and bioactive compound as well as ligands and chiral auxiliaries in asymmetric syntheses. As a consequence, the development of efficient methods for the synthesis of sulfoximines and their functionalizations is greatly needed. However, despite the significant advances made in the functionalization of sulfoximines, only a few examples of 1,2-benzothiazines, which are more attractive pharmacophores as a type of cyclic sulfoximine, have been reported. Herein, we have developed an efficient synthetic method for a wide range of 1,2-benzothia-zines bearing pyridyl as well as carbonyl groups by a rhodium-catalyzed domino C−H activa-tion/cyclization/elimination of alcohol process starting from *S*-aryl sulfoximine and pyridotriazole compounds. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2011-0018355), 2015H1C1A1035955.



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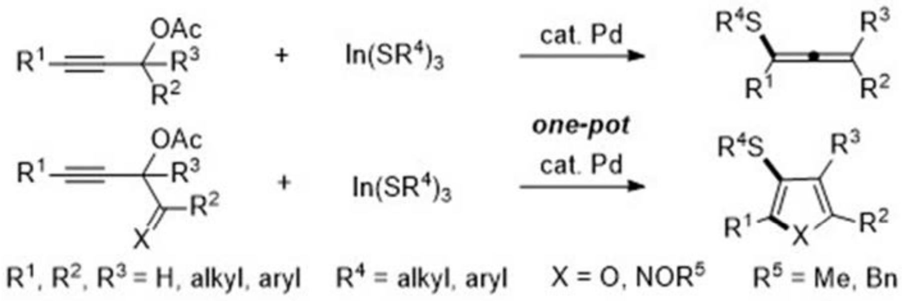
Synthesis of Multisubstituted Allenes, Furans, and Pyrroles *via* Tandem Pd-Catalyzed Substitution and Cycloisomerization

고기훈 한상훈 이필호*

강원대학교 화학과

Recently, an efficient synthetic method towards multisubstituted furans and pyrroles bearing hetero-substituents was reported through metal-catalyzed 1,2-shifts of diverse migrating groups in allenyl systems. However, the introduction of a wide variety of substituents at the 4-position of furans and pyrroles is impossible due to requirement of [1,3]-H shift in these methods. Therefore, the development of an efficient synthetic method for multisubstituted furans and pyrroles bearing 3-heteroatom substituents as well as substituents at the 4-position has been a continuing challenge. Herein, we report Pd-catalyzed propargyl substitution reactions of propargyl acetates with indium organothiolates for the synthesis of multisubstituted allenyl sulfides. This procedure employed tandem Pd-catalyzed propargyl substitution and cycloisomerization reactions from indium organothiolates and propargyl acetates bearing acyl and imidoyl groups for the synthesis of multisubstituted furans and pyrroles in one-pot. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2011-0018355), 2015H1C1A1035955.



☑ ***one-pot tandem reaction***

☑ ***Readily available starting metrials***

☑ ***Highly regioselective***

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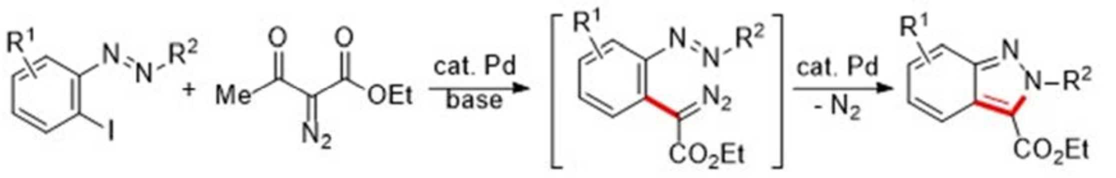
Synthesis of 2*H*-Indazoles *via* Pd-Catalyzed Deacylative Cross-Coupling and Denitrogenative Cyclization from 2-Iodoazoarenes and 2-Iodoaryltriazenes

김지연 백용현 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 denitrogenative cyclization reaction of *in situ* generated diazoacetates having azoaryl and triazenyl aryl moieties in one-pot. Additionally, azoaryl-substituted diazoacetates underwent Pd-catalyzed denitrogenative cyclization to produce 2*H*-indazoles. The present reaction is a good example in which a Pd(0)-catalyst is involved in two catalytic cycles in one-pot. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2011-0018355), 2015H1C1A1035955.



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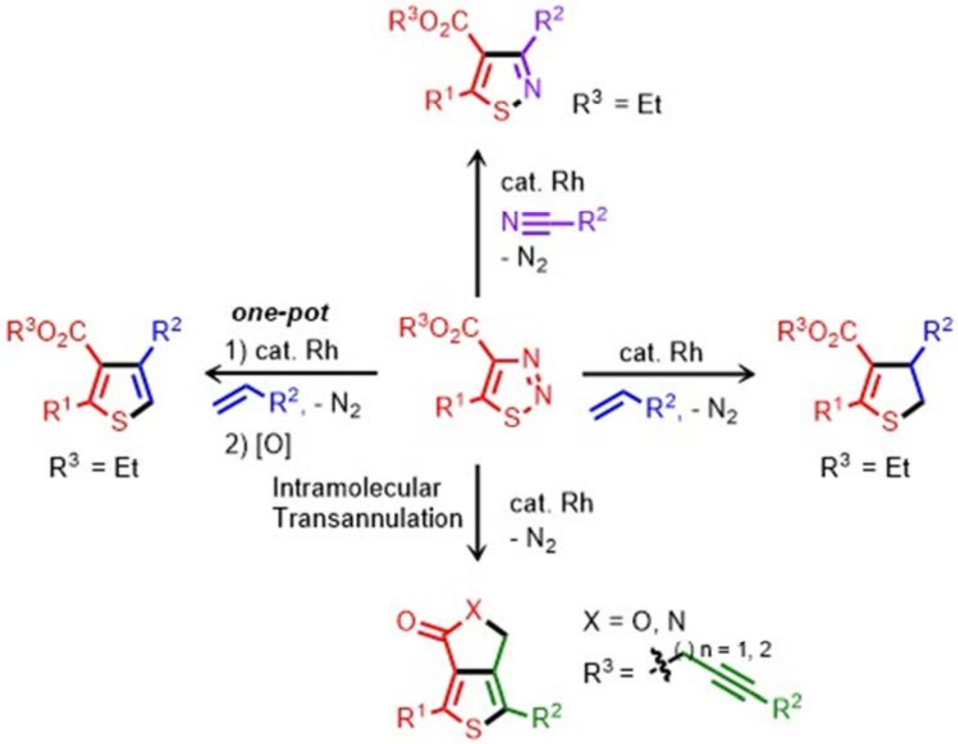
Regioselective Synthesis of Dihydrothiophenes and Thiophenes *via* the Rh-Catalyzed Transannulation of 1,2,3-Thiadiazoles with Alkenes

손정유 김지연 이필호*

강원대학교 화학과

Sulfur-containing five-membered heterocyclic compounds such as dihydrothiophenes and thiophenes represent key structural motifs due to their biological activities in natural products and pharmaceuticals. In addition, thiophene derivatives are very attractive compounds in the field of material science due to their peculiar structural rigidity and useful electronic properties. Thus, the development of synthetic methods for these core scaffolds has received considerable attention in contemporary chemistry. The regioselective introduction of a wide range of substituents onto dihydrothiophene and thiophene rings from readily available starting materials is required. In this study, the regioselective synthesis of a wide range of dihydrothiophenes was developed from the rhodium-catalyzed transannulation of 1,2,3-thiadiazoles with aliphatic, aromatic, and heteroaromatic alkenes. Tandem rhodium-catalyzed transannulation of 1,2,3-thiadiazoles with alkenes followed by 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) oxidation was also demonstrated for the one-pot regioselective synthesis of various thiophenes. This method was employed to efficiently synthesize pentaoligomeric compounds consisting of three benzene and two dihydrothiophene rings. Advantages of the present method include a broad substrate scope, wide functional group compatibility, and high regioselectivity. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIP) (2011-0018355), 2015H1C1A1035955.



R^3O_2C
R^2
R^1
S
N
R^3 = Et
cat. Rh
$N\equiv R^2$
- N_2
one-pot
1) cat. Rh
R^2, - N_2
2) [O]
R^3 = Et
cat. Rh
R^2, - N_2
R^3 = Et
Intramolecular Transannulation
cat. Rh
- N_2
O
X
X = O, N
R^3 =
n = 1, 2

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IONIC INTERLAYER FOR IMPROVED ELECTRON EXTRACTION IN POLYMER SOLAR CELLS

이민수 권태혁[1,*]

UNIST 화학과 [1]UNIST 친환경에너지 공학부

In organic photovoltaics (OPV), interfacial layer are forming a greater part. Electric contact between the active layer and the electrodes largely affect all device-related parameters (JSC, VOC ,and FF) and modification of those interfaces by introducing interfacial layers can change the contact properties to improve the PCE of OPVs. Our team design and inserting new ionic interfacial layer and study the mechanism. We present three Ir-complexes, which has different mobile ions; Li, Na, and K, designed as ionic interlayer. Depending on ions, especially for ionic mobility trend, performances of the devices are dramatically changed in both conventional and inverted structure. Ionic interfacial layer, which has faster ionic mobility, have much higher Power Conversion Efficiency (PCE) than others because of Electric Double Layer (EDL) formation on the interface. Formed EDL helps electron extraction and enhance the JSC and PCE. In this study, we showed the importance of ionic mobility of the interfacial layer materials in electron extraction. Ultraviolet Photoelectron Spectroscopy (UPS) and Conductive Atomic Force Microscope (c-AFM) were applied to analysis the electric double layer formation and effect.

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Molecular Engineering For Enhancement Of Photo/Thermal/Water Stability Of Organic Dyes For Dye-Sensitized Solar Cells

김언영 권태혁[1,*]

UNIST 화학과 [1]UNIST 친환경에너지 공학부

Ru-based sensitizers (N719, N3, black dye and etc.) have been developed continuously and have reached an efficiency of ~11.7% under A.M. 1.5 irradiation. However, these Ru-based sensitizers are not adequate to commercialization because of stability issue and need of thick TiO_2 film for high efficiency. Therefore, we researched 9 organic sensitizers (Fig. 1) changing functional groups (methoxy and carbazole group) and bonds between donor and π-bridge to know which functional groups can enhance the stability and perform high power conversion efficiency at thin TiO_2 film. The 9 sensitizers were basically composed of dithieno[3,2-b:2',3'-d]thiophene (DTT), having robust stability, as a π-conjugated bridge. As a result, TP2 having methoxy groups achieved the highest power conversion efficiency in dithieno[3,2-b:2',3'-d]thiophene (DTT) based sensitizers but stability of TP2 was the worst among the 9 sensitizers. On the other hands, although TP3 showed lower efficiency than that of TP2, TP3 achieved the highest stability against extreme environment. In particular, TP3 showed the strong stability against water because strong hydrophobicity of carbazole groups protected the anchoring groups of sensitizers from water. Finally, photovoltaic and electrochemical properties of 9 sensitizers were measured. Table 1. Shows the photovoltaic parameters of TP series under A.M. 1.5 illumination.

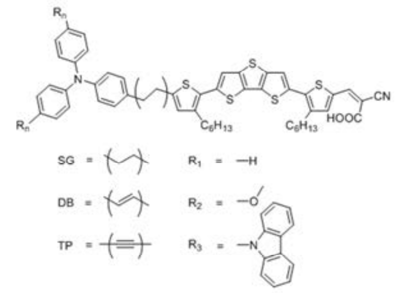

Figure 1. Novel 9 sensitizers based on dithieno[3,2-b:2',3'-d]thiophene (DTT)

	J_{SC} (mA/cm^2)	V_{OC} (V)	FF	Eff. (%)
TP1	14.81	0.73	72.6	7.87
TP2	16.25	0.73	68.6	8.18
TP3	13.44	0.69	72.1	6.66

Table 1. Photovoltaic parameters of TP series

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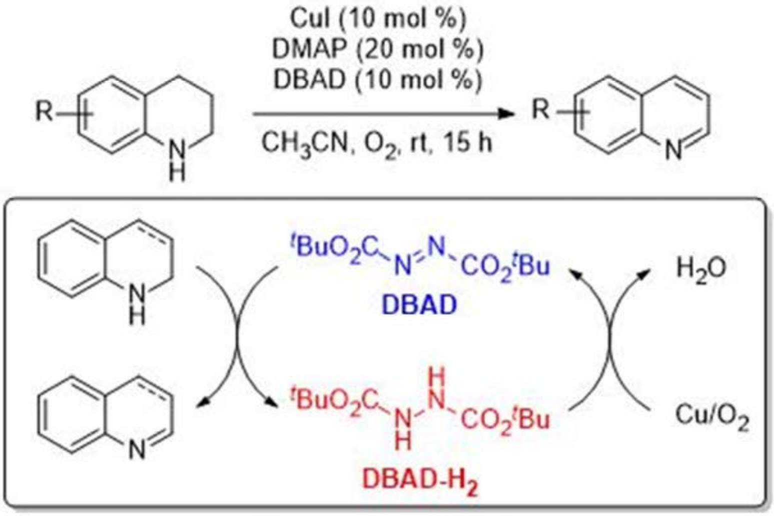
Cu-Catalyzed Aerobic Oxidation of Di-*tert*-butyl Hydrazodicarboxylate to Di-*tert*-butyl Azodicarboxylate and Its Application on Dehydrogenation of 1,2,3,4-Tetrahydroquinolines under Mild Conditions

정다현 김민혜 김진호*

인천대학교 화학과

A new class of co-catalytic system was developed with homogeneous CuI and di-*tert*-butyl azodicarboxylate for aerobic dehydrogenation of 1,2,3,4-tetrahydroquinolines under mild conditions. The developed co-catalytic system is consisting of di-*tert*-butyl azodicarboxylate-mediated dehydrogenation of 1,2,3,4-tetrahydroquinoline and aerobic oxidative regeneration of di-*tert*-butyl azodicarboxylate from di-*tert*-butyl hydrazodicarboxylate using molecular oxygen as a terminal oxidant. A variety of quinolines were efficiently synthesized by the developed Cu and di-*tert*-butyl azodicarboxylate co-catalytic system.



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Synthesis and evaluation of dimerized novel imaging ligands for prostate cancer

권영도 김희권[1,*]

전북대학교 의과학과 [1]전북대학교 의학전문대학원/핵의학교실

Prostate cancer is one of common cancers which diagnosed in men. Prostate-specific membrane antigen (PSMA) is known as an imaging target for prostate cancers because PSMA is highly upregulated in the primary cancers and metastases. In the present study, we prepared novel dimerized PSMA inhibitors containing urea unit. Also, the ligands were attached with an imaging agent such as cyanine dye in order to improve ability to detect prostate tumor. Biological evaluations suggest that novel dimerized inhibitors were more potential agents applicable for diagnosis of prostate cancer.

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Electronically tuned through Bond Energy Transfer Up-Conversion Pyrene-phenylthiazole Donor-Acceptor Dyad : Sensing and Biological Applications

허준혁 조효이[1] 김홍석[1,*]

경북대학교 응용화학 [1]경북대학교 응용화학과

A 2-(2’-hydroxyphenyl)-4-pyrenyl-thiazole based probe (Probe 1) was designed and synthesized. Probe 1 showed extensively high fluorescence emission intensity centered at 425 nm in DMSO. And showed excimer emission centered at 495 nm in DMSO-Glycerol system (1:9 v/v). Higher emission intensity at 425 nm in DMSO resulted from effective intra-molecular charge transfer (ICT) coupled energy transfer (ET) from pyrene unit to phenylthiazole unit through the structurally bent rigid conformation. In contrast in DMSO-Glycerol system (1:9 v/v) simultaneous inhibition of ICT-ET occurred from pyrene to phenylthiazole unit with effective stabilization of inter-molecular pyrene units excimer-exciplex complex through the aggregated phenomenon resulted in excimer emission. Further sensing ability of 1 towards anions and its biological applications also demonstrated.

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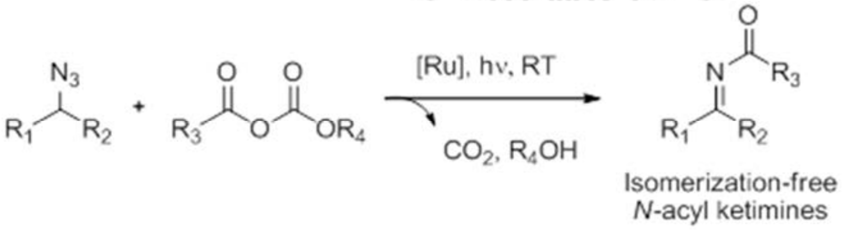
Selective Synthesis of *N*-Acylimines by the Reaction of N-H Imines with Acyl Alkyl Carbonates

권예랑 이영호* 박재욱*

POSTECH 화학과

N-Acylimines are important intermediates in organic synthesis, which have electron-withdrawing acyl substituents to overcome the low electrophilicity and limited utility of *N*-alkylamines and *N*-arylamines. They have been utilized in numerous C-C and C-heteroatom bond forming reactions. However, *N*-acylimines are known to be too unstable to be stored and easily tautomerized to corresponding enamide. Thus, they are generally prepared in situ for the reaction with nucleophiles. We synthesized various *N*-acylketimines including enolizable aliphatic ones from the alkyl azides in a one-pot procedure. And we demonstrated the utility of cyclic *N*-acyl ketimine in nucleophilic addition of Grignard reagent to afford acetamide with high diastereoselectivity.



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A Tin-Free Route to trans-Diels−Alder Motifs by Visible Light Photoredox Catalysis

이준희* 모선일[1]

동국대학교 신소재화학과 [1]아주대학교 에너지시스템학부 화학

Stereoselective construction of trans-fused bicyclic systems is an important task in organic synthesis, because they are among the most versatile intermediates for the synthesis of various polycyclic natural products and relevant compounds. Danishefsky and co-workers developed a two-step trans-Diels− Alder (DA) protocol, which provides expeditious access to trans-fused octalins and hydrindanes from nitroalkene dienophiles and simple dienes. This conceptually novel strategy involves equipping cyclohexenes with a nitro group as a traceless activating group, thereby enhancing the dienophilicity of the otherwise unreactive dienophiles to yield cis-fused DA adducts. Subsequent free radical-mediated reduction of this angular functionality using AIBN and tributyltin hydride furnishes the target trans-fused bicyclic systems with good to excellent selectivity. The research groups of Danishefsky and Yamamoto have independently reported that the Lewis acid catalyzed DA reactions of α-halogentated 2-cycloalkenones with 1,3-butadienes can provide efficient access to cis-fused bicyclic systems with a halogenated quaternary stereogenic center. The halogenated cis-fused cycloadducts were then successfully converted to the trans-fused octalones in a highly stereoselective fashion by tin-mediated free radical reduction and reductive alkylation. Despite these advances, there still exists a need for developing new and green methods for the stereoselective synthesis of trans-fused polycyclic systems, because organotin hydride-mediated radical reactions have two major disadvantages: the intrinsic toxicity of tin-based reagents and the difficulty of removing their residues from the products. We envisaged that visible-light-induced photocatalytic dehalogenation might be an ideal platform for the development of a green and environmentally benign trans-DA protocol that is free of organotin reagent. This presentation will deal with the full details of this novel reaction.


O
Br
R
R
H
R'
Ru(bpy)$_3$Cl$_2$
Hantzsch ester
nBu$_3$N, DMSO
blue LEDs, rt
up to 96% yield
up to >99% dr

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장소: 일산 KINTEX
발표코드: **ORGN.P-240**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An Efficient Amidation of Aldehyde Using Bromo group at Room Temperature

김희권

전북대학교 의학전문대학원/핵의학교실

Amide unit is commonly found in a lot of biopharmaceuticals, natural compounds, and polymer. The Amide unit has been utilized to a variety of fields such as plastics, dyes, pharmaceuticals synthesis. The amidation of aldehyde is one of efficient and direct methods for the preparation of amide bonds. However, most of synthetic methods have used harsh reaction condition. Herein, novel and mild synthetic method for the amidation of aldehyde is described. In the novel protocol, aromatic and aliphatic aldehydes were treated with bromo compound for activating aldehydes, and were readily converted the corresponding amides with high yields at room temperature.

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Blue emitters based on benzo[*g*]quinoline derivatives for Organic Light Emitting Diodes

조석원 김창민 강지수 윤승수*

성균관대학교 화학과

We designed and synthesized two emitters based on benzo[*g*]quinooline derivatives for Organic Light-Emitting Diodes. To examine their electroluminescent (EL) properties, the organic light emitting diodes (OLEDs) devices using two materials as emitters were fabricated with the following sequence; indium-tin-oxide (ITO) / 4,4′,4″-Tris[2-naphthyl(phenyl)amino]triphenylamine (2-TNATA) (30 nm) / N,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) (20 nm) / Blue emitters (30 nm) / bathophenanthroline (Bphen) (30 nm) / lithium quinolate (Liq) (2 nm) /Al (100 nm). All devices showed the efficient emissions.

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Tau tangle-specific Near-Infrared Fluorophores

서진호 박근영 구세영 정태호 김수빈 김종승*

고려대학교 화학과

Tau proteins are important in stabilizing microtubules by electrostatic attraction. Tau proteins are expressed in the neurons of adults, ranging from 352 to 441 amino acids in length.By hyper phosphorylation, tau proteins disassemble from microtubules and self-aggregate.It can be accumulated, resulting Nero Fibrillary Tangle (NFT) in the human brain. This NFT is the main cause of Alzheimer disease by interrupting neurons interaction. Detection of Tau tangle is essential in understanding and detecting Alzheimer disease.

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Enzyme triggered theranostics

신원섭 서진호 심인섭 박근영 선우경 손수빈 정태호 김종승*

고려대학교 화학과

The development of targeted and effective theranostic (therapeutic and diagnostic) chemotherapeutic agents is highly desirable for precise diagnosis and treatment of cancer. To realize this goal, we developed a cancer-targeting and enzyme-triggered theranostic prodrug 1, containing 7-ethyl-10-hydroxycamptothecin (SN-38), a well-known anticancer drug, which inhibits topoisomerase I in the cell nucleus; hydroquinone as an enzyme-triggered moiety; and biotin as a cancer targeting unit. Enzyme-triggered theranostic prodrug 1 selectively targets cancer cells and is subsequently activated in the presence of NAD(P)H: quinone oxidoreductase-1 (NQO1), a cytosolic flavoprotein that catalyzes the two-electron reduction of quinone moieties with the concomitant consumption of NADH or NADPH as electron donors. High levels of NQO1 were found in a variety of cancer cell lines compared to healthy cells, and therefore, it is an excellent target for the development of cancer targeted drug delivery systems. Upon preferential cancer cell delivery and uptake, aided by biotin, the enzyme-triggered theranostic prodrug 1 is cleaved by NQO1, with the subsequent release of SN-38, inhibiting topoisomerase I, leading to apoptosis. The drug release and induced apoptosis of cancer cells expressing both biotin receptors and high levels of NQO1 was simultaneously monitored via the innate fluorescence of the released SN-38 by confocal microscopy. In vitro and in vivo studies showed an effective inhibition of cancer growth by the enzyme-triggered theranostic prodrug 1. Thus, this type of enzyme

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COX-2 Targeted Drug Delivery System

박근영 신원섭 김수빈 구세영 서진호 김종승*

고려대학교 화학과

The targeted theranotic agent has been the focus on the cancer treatment to minimize side effect in recent years. To achieve this goal, we developed a cancer-targeting and enzyme-triggered theranostic prodrug 1, containing 7-ethyl-10-hydroxycamptothecin (SN-38), a well-known anticancer drug, which inhibits topoisomerase I in the cell nucleus; ester bond as an enzyme-triggered moiety. Enzyme-triggered theranostic prodrug 1 selectively targets COX-2 which is overexpressed in cancer cells. The prodrug is subsequently activated in the presence of esterase which is a hydrolase enzyme that splits esters into an acid and an alcohol in a chemical reaction with water called hydrolysis and therefore, it is an excellent target for the development of cancer targeted drug delivery systems. Upon preferential cancer cell delivery and uptake, aided by COX-2 inhibitor, the enzyme-triggered theranostic prodrug 1 is cleaved by esterase, with the subsequent release of SN-38, inhibiting topoisomerase I, leading to apoptosis.

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Mitochondria targeted combinational therapy

신원섭 선우경 정태호 심인섭 서진호 손수빈 김종승*

고려대학교 화학과

We report on a mitochondria-specific combinational theranostic agent 1. This system contains a chlorambucil prodrug and an aggregation induced emission dye. In addition, compound 1 bears both an intracellular thiol-triggered moiety and a mitochondria targeting unit (triphenylphosphonium). Glutathione (GSH), is the most abundant thiol and its concentrations are significantly higher in a great number of cancer cells lines, compared to normal cells. The GSH-induced prodrug 1 activation releases chlorambucil and reveals a mitochondria targeted aggregation induced emission (AIE) fluorescence, resulting in cell apoptosis via the caspase pathway due to mitochondrial dysfunction.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Cancer theranostic agent towered mitocondria

신원섭 김원영 박근영 김수빈 구세영 김종승*

고려대학교 화학과

Tissue selective targeting and specific suborganellular localization combined with an efficient pathology associated enzymatic activation of drugs in drug delivery systems may exhibit a clear advantage over conventional cancer treatment. Here, a mitochondria targeted aggregation induced emission (AIE) fluorophore further conjugated with an DT-Diaphorase cleavable masking unit showed preferential uptake in cancer cells and was selectively activated, resulting in bright AIE fluorescence and apoptosis via the caspase pathway, triggered by mitochondrial dysfunction. In vivo experimental data further support the conclusions from in vitro experiments, clearly showing the dependence of the therapy's success on both the suborganelle localization and specific in situ activation. And the site specific and enzyme dependent activation and aggregation was further supported by in vivo and ex vivo imaging. As a whole, the data comprised in this work represent a strong argument for the further development of this type of novel anticancer drugs.

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Tumor targeted phototherapeutic agent

<u>신원섭</u> 손수빈 김형석 김원영 김종승*

고려대학교 화학과

Photolabile protecting groups are a versatile tool to trigger reactions by light irradiation. Using nitrovanilin, herein, we designed, synthesized and evaluated therapeutic efficacy of a novel photo-cleavable and targeted phototherapeutic. The nitro group of nitrovanilin has both light-activating properties and quenching effect for the fluorophore. On the other hand, the presence of biotin group specifically guide the phototherapeutic to the cancer cells compared to normal cells. Upon irradiation of light (by a 405 nm laser), the nitrobenzyl group of phototherapeutic is cleaved, resulting in release of anticancer drug (SN38), which can be observed by fluorescence changes of activated SN38. Using this strategy, it is possible not only to control of the drug release but also monitoring the site of activation and distribution of drug by fluorescence changes. Before irradiation, the phototherapeutic have no toxicity, however, after irradiation, it shows high cytotoxicity against A549 cells, in vitro and in vivo. Thus, on demand photo-cleavable phototherapeutic can provide a fascinating platform for selective targeting of cancer cells and site specific release of drug that decrease the side effects of the chemotherapy

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장소: 일산 KINTEX

발표코드: **ORGN.P-248**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Sensing Proteins using Light up – Aggregation Induced Emission (AIE)

최후연 김상필[1] 이승호[2] 유자형[3,*]

UNIST Chemistry [1]UNIST 분자과학부 [2]UNIST 화학과 [3]UNIST 자연과학부 화학과

The concentration of proteins is significantly related to specific diseases for early diagnosis. Until now, protein sensing requires high chemistry, technologies and expensive cost. In here, proteins can be detected and identified by five aggregation induced emission luminogens (AIEgens) using arrays depending on affinity between different functional groups of AIEgens and proteins. Fluorescence patterns will be classified using six proteins such as BSA, transferrin, fibrinogen, β-galactosidase, esterase and acid phosphatase and five AIEgens. In absence of proteins, water-soluble AIE molecules which have six functional groups showed little fluorescence. This is because the AIE molecules can freely rotate and show no fluorescence in soluble solvent. However, in presence of proteins, the interaction with six proteins and functional groups provide distinct fluorescent response patterns because AIE molecules cannot rotate freely and interact with specific proteins showing high fluorescence due to restriction of rotation from intramolecular hydrogen bonding and binding with proteins with two sides. Depending on different fluorescence response, the linear discriminant analysis (LDA), the statistical analysis, can be successfully used to identify the proteins with high accuracy

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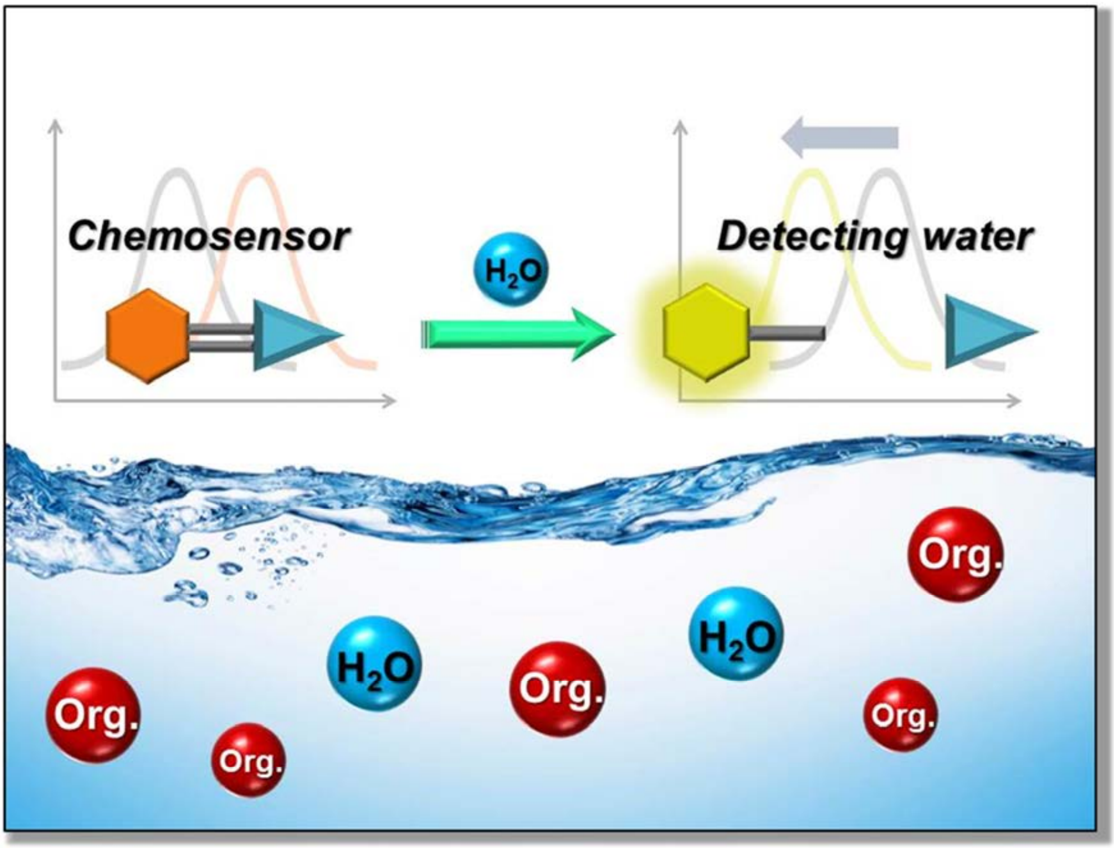
Coumarin-based Moisture Sensor Triggered by Schiff Base Hydrolysis for the Fluorescence Detection of Water in Organic Solvents

김원영 신진우 심인섭 손수빈 정태호 김종승*

고려대학교 화학과

A Chemodosimeter based water sensor was designed and developed for the detection of water inorganic solvents. The coumarin based Schiff base was found to be an excellent indicator of moisture, via rapid in situ hydrolysis. It showed the prompt optical change upon hydrolysis with water. And also, a structure-relationship examination of a small library of Schiff bases revealed the critical importance of hydrogen bond acceptors in close proximity to the imine bond, and this observation was further supported by theoretical calculations as well as the solid state structure analysis. The most sensitive compound demonstrated a limit of detection and quantification of 0.18% and 0.54% v/v water in DMSO, respectively.


Chemosensor
H_2O
Detecting water
Org.
H_2O
Org.
H_2O
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장소: 일산 KINTEX

발표코드: **ORGN.P-250**

발표분야: 유기화학

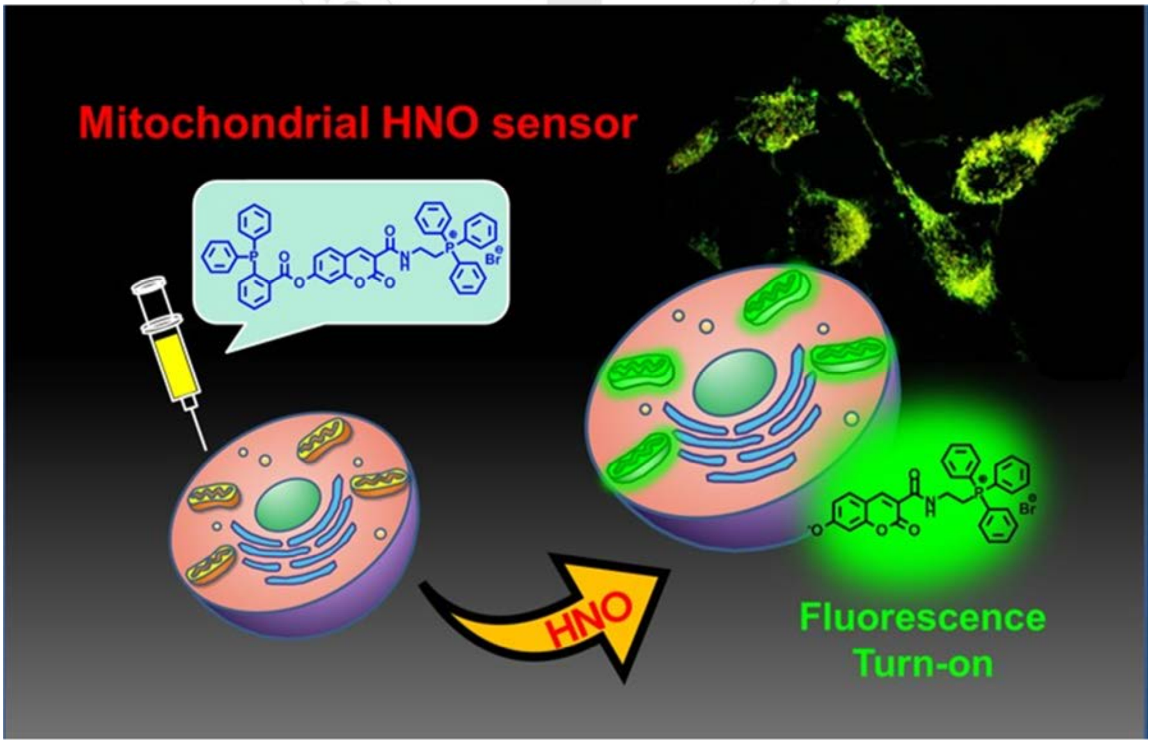
발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly Sensitive Bioorthogonal Two-photon Fluorescence Sensor for Detecting Mitochondrial HNO Formation

선우경 서진호 심인섭 구세영 김원영 김종승*

고려대학교 화학과

A bioreductant-resistant ‘turn-on’ chemodosimeteric Staudinger reaction based1 fluorescent probe Mito-1 has been developed for the detection of mitochondrial HNO in live cells. Mito-1 enables to detect HNO as low as to ~18 nM. It has the capability to detect both exogenous and endogenous mitochondrial HNO formation in cellular milieus by providing fluorescence images. Its two-photon imaging ability fosters its use as a noninvasive imaging tool for detection of mitochondrial nitroxyl.



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장소: 일산 KINTEX

발표코드: **ORGN.P-251**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

An Indomethacin Guided Ratiometric Fluorescent Chemosensor for Cancer Recognition and Diagonosis

김형석 구세영 신원섭 서진호 심인섭 김수빈 선우경 김종승*

고려대학교 화학과

Cyclooxygenase-2 (COX-2) is a promising candidate of cancer recognition target, as it is highly expressed in tumour cells, but barely in the normal cells. Thus, as an inhibitor of COX-2, indomethacin (IMC) has great potential to be an efficient guiding unit for tumor visulization and diagonosis. In this regard, we designed and synthesized an IMC conjugated fluorescent chemosensor, IQR-1, which is able to present ratiometric fluorescent response toward biothiols in living systems. IQR-1 successfully discriminates between human carcinoma and normal cells by measuring GSH levels in living cells, which suggests that it represents a promising cancer specific marker for early diagnosis of tumor.

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발표분야: 유기화학
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In-Situ Generated Fluorescent- Zn2+-anthracene Ensemble for Selective Detection of 2,4,6-trinitrophenol in 80% Aqueous DMSO

Anup Pandith 서한솔[1] 김홍석*

경북대학교 응용화학과 [1]경북대학교 응용화학공학부 응용화학전공

Highly selective in situ generated divalent Zn2+●anthracene complex based probe was designed for sensing 2,4,6-trinitrophenol (TNP) in environmentally more benign and biocompatible medium. In situ generated highly fluorescent chelated Zn2+●P (1:1) complex detected TNP more selectively through switch-off response with very high Stern-Volmer quenching constant (Ka = 3.75 x 106 M-1) in 1:1:2 stoichiometry in 80% aqueous medium. Selective quenching response occurred with TNP is due to the effective destruction of chelated complex through the efficient protonation at secondary amine there by causing effective resonance energy transfer (RET) from anthracene unit to latter. Thus produced P2+●(TNP)-2 complex showed anthracene monomer band quenching resulted from efficient RET, accompanied through the synergistic multiple hydrogen bonding, electron rich-electron deficient An-TNP interactions and columbic interactions. Applications were demonstrated through the ensemble coated hydrogel (ECH) UV assisted naked eye sensing. The lowest detection limit for TNP was 3.01 x 10-10 M in 80% aqueous DMSO.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

A neuron ER stress targeting NIR and MRIcontrast agents penetrating blood brain barrier

심인섭 구세영 정태호 손수빈 김수빈 김종승*

고려대학교 화학과

We report here a blood brain barrier penetrating NIR and MRI contrast agents targeted at neuron ER stress. Our NIR and MRI contrast agents are conjugated with dieckol via the click reaction. Dieckol is a natural polyphenol isolated from several brown algae that have reportedly shown antioxidant, anti-inflammatory, and neuroprotective activities. Compared with the fluorophore alone, the target compound (Cy7-DE) showed much better BBB penetrating ability and brain cell permeability. These results support our earlier work on the dieckol scaffold and provide further evidence for its remarkable function as a BBB transport ligand and ER stress suppressor. Future work will entail the study of the Gd-complex-conjugated dieckols to further probe the performance of this ligand, thus opening the way for brain-specific MRI contrast agents for simultaneous monitoring and treatment of a large variety of neurodegenerative diseases.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

A non-enzymatic approach to sensing uric acid in blood serum : complementary H-Bonding on a BODIPY scaffold

신진우 정태호 김원영 박근영 손수빈 선우경 김종승*

고려대학교 화학과

Uric acid is a major metabolite of purine base nucleic acids. Normal uric acid concentrations in blood serum fluctuate between 120 and 380 µM, whereas perturbed concentrations are indicative of a wide variety of diseases, such as hypertension, cardiovascular disease, kidney disease and certain types of cancer. The reliable detection of this metabolite as a biomarker for these diseases is highly important, especially since elevated levels of uric acid have been linked to increased risk of kidney failure. The current methods employ a relatively costly uricase enzymatic assay or electrochemical methods, and suffer from drawbacks due to interference by ascorbic acid present in relatively high concentrations in blood serum.The current work describes a novel non-enzymatic approach to the detection of this biomarker by a BODIPY fluorophore, with the fluorescence quenched by a PET process with an appended ligand. The ligand was rationally designed to exhibit a complementary hydrogen donor acceptor pattern leading to hydrogen bonded uric acid, and thus the selective binding of uric acid leads to the inhibition of the PET process, resulting in bright fluorescence.Our probe was able to detect a wide range of biologically relevant concentrations (60 – 700 µM) in blood serum and showed good selectivity over other competing biological compounds. Thus our probe could represent a major cost-effective advancement over the currently used methods.

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장소: 일산 KINTEX
발표코드: **ORGN.P-255**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

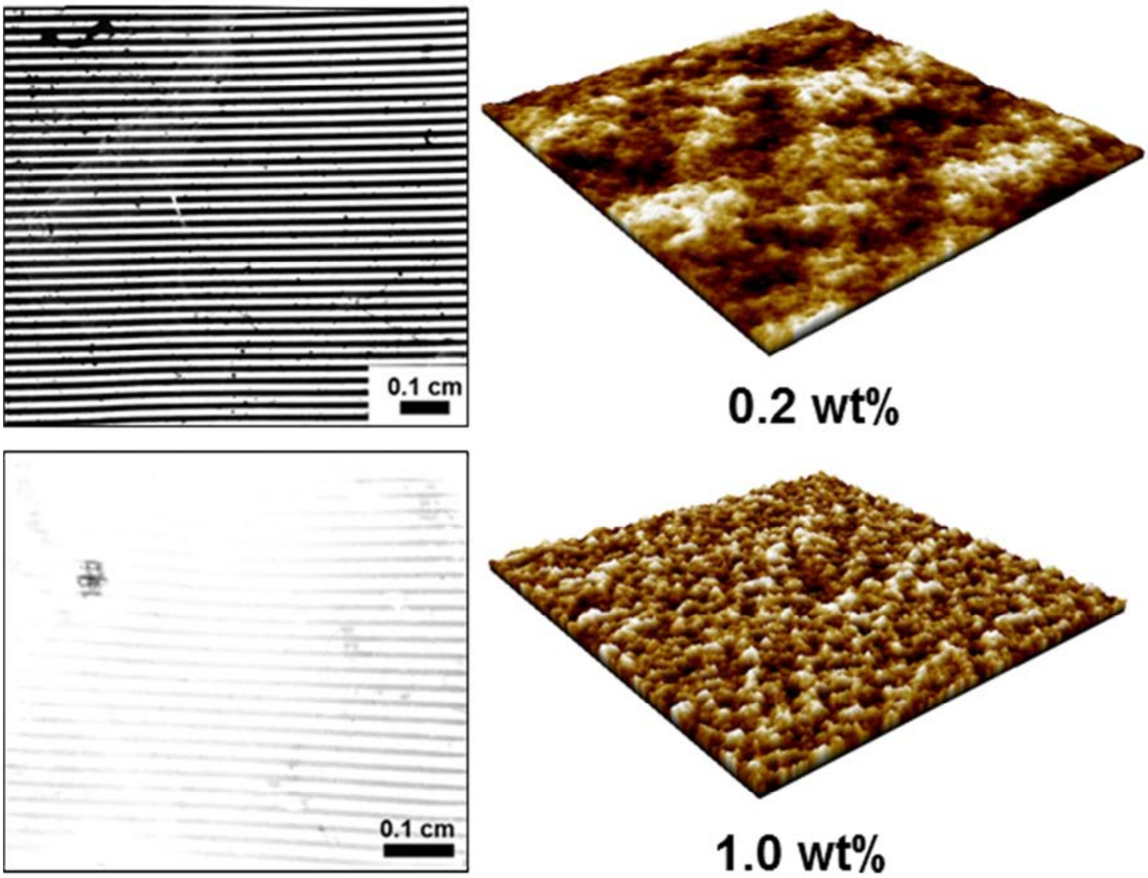
Systematic Study of Functionalizable, Non-Biofouling Agarose Films with Protein and Cellular Patterns on Glass Slides

한경엽 고상원[1] 이정규*

경북대학교 화학과 [1]한국철도기술연구원 교통환경연구팀

We demonstrated a systematic investigation on chemically functionalizable, non-biofouling agarose films over large-area glass surfaces. Agarose films, prepared with varying concentrations of agarose (aq), were activated by periodate oxidation to generate aldehyde groups at the termini of agarose chains. The non-biofouling efficacies and binding capabilities of the activated films were evaluated using protein and cellular patterning, assisted by a microarrayer, microcontact printing, and micromolding in capillaries. The characterization of a fluorescence slide scanner and a scanning probe microscopy revealed that the pore sizes of the agarose films played an important role in achieving desirable film performance: the 0.2 wt% agarose film exhibited the optimum efficacy in this work.

Protein Patterns on Agarose Films



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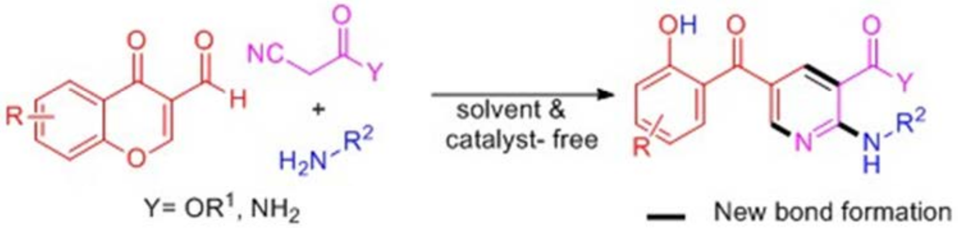
발표코드: **ORGN.P-256**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Substituted 2-Aminopyrinides by Catalyst- and Solvent-Free Thermal Multicomponent Approach

BARALEKRAJ 이용록*

영남대학교 화학공학부

Pyridines are the most common and fundamental N-containing heterocyclic compounds found in many natural products and active pharmaceuticals. Among these, 2-aminopyridine derivatives are found widely in pharmaceutical drugs and bioactive materials. These 2-aminopyridine-based molecules have a wide range of biological properties, such as anti-inflammtory, antimalarial, CB_2 agonist, CRF_1 receptor antagonist, BMP inhibitory, CDK8 inhibitory, and nNOS inhibitory activities. In addition, they are used widely as the building blocks for the synthesis of drug leads and biologically interesting materials.Owing to their important biological and pharmaceutical applications, several synthetic approaches to the construction of 2-aminopyridines based on transition-metal catalyzed and metal-free reactions have been developed. Typical methods include the transition-metal catalyzed amination of 2-halopyridines with substituted/unsubstituted amines or ammonia, $HSiCl_3$-mediated reduction of aromatic nitro compounds, and amination of pyridine *N*-oxides with the corresponding amines or isocyanides. Here, we present synthesis of a range of polysubstituted 2-aminopyridine derivatives by using thermal multicomponent cascade reaction from readily available 4-oxo-4*H*-chromene-3-carbaldehydes with cyanoacetates or cyanoamide and anilines or primary amines under solvent and catalyst-free conditions (Scheme 1). As an application of this methodology, the antibacterial activities of some of the synthetic compounds were evaluated.



Scheme 1. Solvent and catalyst-free synthetic approach for substituted 2-aminopyridines.

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장소: 일산 KINTEX

발표코드: **ORGN.P-257**

발표분야: 유기화학

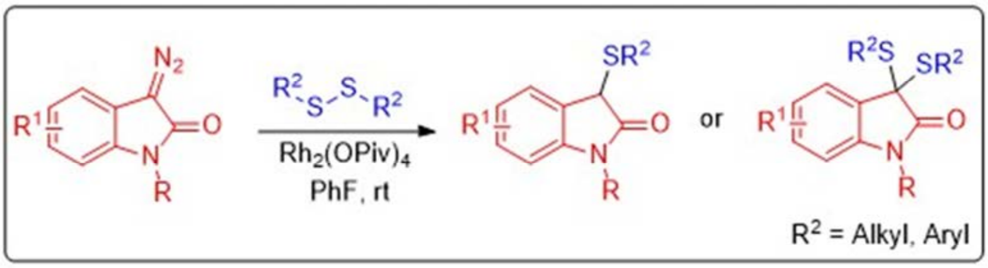
발표종류: 포스터, 발표일시: 목 11:00~12:30

Rhodium (II)-Catalyzed Direct Sulfenylation of Diazooxindoles with Disulfides *via* C-S Bond Formation

<u>KHANALHARIDATTA</u> 이용록*

영남대학교 화학공학부

3-Substituted oxindoles are found widely in naturally occurring and bioactive synthetic molecules. Among these, oxindoles bearing heteroatoms as substituents at the C3 position are particularly important and useful in medicinal chemistry. 3-Sulfenyloxindoles have attracted considerable attention as leading pharmaceutical compounds owing to their important biological activities and properties. Recently, they are used as building blocks for the asymmetric synthesis of biologically interesting 3-sulfenyl substituted quaternary stereocenters. Although several synthetic methods for the synthesis of 3-sulfenyloxindoles have been developed, more environmentally benign and efficient arsenals are in strong demand for improving the reaction steps. Therefore, the need to develop new and simpler synthetic methods for 3-sulfenyloxindoles prompts this study relying on the characteristic reactivity of diazo compounds. This study reports one-pot synthesis of biologically interesting 3-alkylthiooxindoles, 3,3-dialkylthiooxindoles, or 3,3-diarylthiooxindoles by Rh(II)-catalyzed reactions of readily available diazooxindoles with a range of disulfides (Scheme 1). The transformation is proposed to proceed through sulfur ylide formation followed by S-S bond cleavage of disulfides and a rearrangement reaction.



Scheme 1. Our strategy for the synthesis of 3-sulfenyloxindoles or 3,3-disulfenyloxindoles.

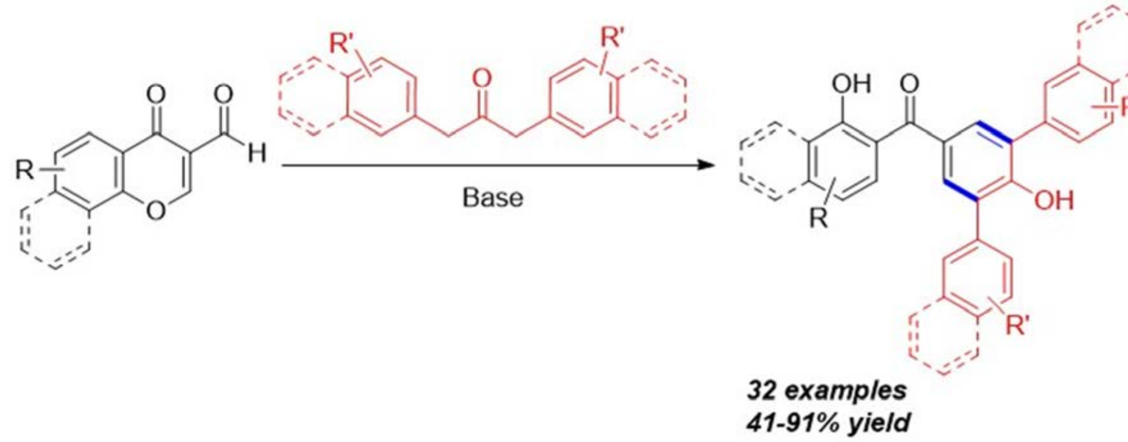
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-258**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Facile Route to Benzophenones bearing *m*-Terphenyls and Their Application as Promising UV-Filters

TAMARGO RAMUEL JOHN 이용록[1,*]

영남대학교 화공관 [1]영남대학교 화학공학부

Molecules bearing terphenyl moiety are widespread in nature and possess a broad range of biological activities. In recent years, *m*-terphenyls have gained considerable attention for its promising properties such as anticancer, anti-apoptotic, anticoagulant, neuroprotective, and cytotoxic activities. In addition, they have been extensively employed in advanced materials such as low-density self-assembled monolayers (SAM), polymer-based photovoltaic cells, organic field effect transistors, and liquid crystals for organic light-emitting diodes (OLED due to its highly conjugated π-systems.Owing to their importance and usefulness, a number of synthetic routes to access terphenyls based on aryl–aryl coupling reactions and benzannulation reactions have been developed. However, there is still high demand for more facile and efficient arsenals to overcome the necessity of complex and expensive transition metal catalysts as well as harsh reaction conditions. Herein, we describe a transition-metal-free [3+3] cycloaddition reaction for the synthesis of polyfunctionalized *m*-terphenyls in good to excellent yield starting from readily available substrates under a mild base (Scheme 1). As an application, the synthesized compounds were evaluated for UV absorption properties. In vitro study shows that majority of the compounds can be classified as broad spectrum UV-filters with high absorption coefficients.



Scheme 1. Our strategy for the construction of diverse m-terphenyls.

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발표분야: 유기화학
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2'-Deoxyuridines labeled with a fluorene derivative: pH-sensitive probes for SNP discrimination

황준연 황길태*

경북대학교 화학과

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. Recently, we reported two fluorescent 2´-deoxyuridines, U^{AF} and U^{DAF}, labeled with 2-aminofluorene and 2-dimethylaminofluorene units, respectively, and having values of pKa of 4.27 and 4.66, respectively, display “turn-on” emission responses in acidic solutions. Herein, we have synthesized oligodeoxynucleotides (ODNs) bearing the 2’-deoxyuridine labeled with a fluorene derivative as a pH-sensitive SNP probe. Thermal stability, structural information and fluorescence property of ODNs under different pH conditions will be discussed.

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A Highly Regioselective Synthesis of 3-Arylindoles from Anilines and Styrenes

고태윤 윤소원*

한양대학교 화학과

Due to their unique biological properties, the construction of indole framework is attractive target in organic synthesis and of considerable importance. In particular, 3-arylindoles are important scaffolds in natural products, pharmaceuticals and functional materials. Even if various methods for the construction of 3-arylindoles have been reported, new and more efficient synthetic strategies still continue to be pursued. Herein, we report the development of Pd-catalyzed intermolecular dehydrogenative coupling reaction between styrenes and *N*-Ts-anilines for the synthesis of 3-arylindoleswith high efficiencyand regioselectivities.

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발표분야: 유기화학
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Sequential NHC/Rh(III)-Catalyzed One-Pot Synthesis of Phthalides and Isocoumarins

유현지 윤소원*

한양대학교 화학과

One-pot synthesis is a powerful strategy to increase the ability of chemical reactions which reduces the reaction time and improves the product results. It is also a greener chemistry synthesis which is avoiding a several separation procedure and further purification as well. The combination of organocatalysts, especially N-heterocyclic carbenes (NHCs), and transition metal catalysts is highly attractive with great potential, which may lead to new reactivity and high efficiency. Due to the good ligating ability of NHCs for transition metals, however, only few examples on the successful merger of NHC and transition metal catalysis have been reported with limited and specific scope. Although significant advances have been made in NHC catalysis and transition metal-catalyzed C-H activation individually, to the best of our knowledge, their merger has not been reported so far. Herein we report our recent results of the investigations into one-pot sequential catalysis merging NHC catalysis and Rh^{III}-catalyzed C-H activation, leading to the formation of phthalides and isocoumarins.

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The effect of triphenylamine moieties on diketopyrrolopyrrole dyes to aggregation induced emission enhancement

황태규 김재필[*] 노정우[1] 우성윤[2] 이재문[2]

서울대학교 재료공학부 [1]서울대학교 공과대학 재료공학부 [2]서울대학교 재료공학과

Aggregation induced emission enhancement(AIEE) is an interesting phenomenon for organic luminophores. Most organic compounds have a planar structure and higher photoemission efficiency in solution than in solid states. However, some organic luminophores have rotation groups which consume energy after they are excited in solution. When these luminophores crystallize and the free rotation of groups is restricted in solid state, the photoemission efficiency becomes higher than in solution. In this study, four red emitting dyes were synthesized, two were previously reported and the other two were newly synthesized. The dyes contained different structural types of triphenylamine (TPA) moieties. All synthesized dyes in this study showed AIEE dynamics. Especially newly synthesized dyes (D6C-DBP2, D6C-DBP1) showed red fluorescence in solution state as well

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발표종류: 포스터, 발표일시: 목 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.

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A new anion receptor based on naphthalimide

<u>김정현</u> 김성국*

경상대학교 화학과

A strapped calix[4]pyrrole has been synthesized as a fluorogenic sensor for anions. In this case, the naphthalimide was introduced into the strap as a signaling unit. UV/vis, fluorescence and ^{1}H NMR spectroscopic analyses revealed that this calix[4]pyrrole is able to bind various kinds of anions accompanying significant color and fluorescence changes. High selectivity for the fluoride and chloride anion was shown by this anion receptor.

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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 lithium halide ion pairs highly selectively over other akali metal salts.

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KF and CsF Recognition and Extraction by a Calix[4]crown-5 Strapped Calix[4]pyrrole Multitopic Receptor

김승현 김성국*

경상대학교 화학과

A calix[4]crown-5 strapped calix[4]pyrrole multitopic receptor was synthesized on the basis of a calix[4]arene and calix[4]pyrrole hybrid compound. In this case, the calix[4]arene subunits was locked in the con or 1,3-alternate conformation whereas the calix[4]pyrrole constituent is conformationally flexible. It was found by 1H NMR spectroscopic analyses that the ion pair receptor is able to bind specific ion pairs such as potassium and cesium salts highly selectively. In these cases, 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 crown-5 moiety or the diethylene glycol linker.

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A Heterotritopic Ion Pair Receptor Based on Calix[4]pyrroles and a Poly Ether

최한별 김성국*

경상대학교 화학과

A new heterotritopic ion pair receptor was synthesized. The receptor is comprised of two calix[4]pyrroles as anion binding units and poly ethers as a cation binding unit. From now on ^{1}H NMR spectroscopic analyses showed that, upon exposure to certain ion pairs, the poly ether encompasses cations bringing the two calix[4]pyrrole in proximity. This facilitates cooperate anion binding of the two calix[4]pyrrole units.

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A solid-phase synthetic method for combinatorial production of *N*-alkyl-4-alkylamino-1-aryl-1*H*-pyrazolo[3,4-*d*]pyrimidine-6-carboxamide library

허윤정 전문국[1,*]

고려대학교 화학과 [1]한국화학연구원 의약화학연구센터

Solid-phase organic synthesis (SPOS) provides an efficient synthetic route to small organic molecule libraries. It is comprised of i) attachment of a synthetic intermediate onto a solid support, typically polymeric support, through a linker, ii) repeated reactions on solid phase, filtration, and washing, and iii) cleavage from the solid support to afford the desired final product. Reactions on solid phase can be driven to completion by use of excess reagents and supported intermediates can be purified by simple filtration and washing. Therefore, SPOS can adapt to automation and mix-and-split synthesis is possible. 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. The novel solid-phase synthetic method would serve as a combinatorial route to *N*-alkyl-4-alkylamino-1-aryl-1*H*-pyrazolo[3,4-*d*]pyrimidine-6-carboxamide library.

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Synthesis of Layered Dendrimers via Click Chemistry

도우미 이재욱*

동아대학교 화학과

The well-known click chemistry which is useful tool for synthesis of dendrimers, is a Cu(I)-catalyzed azide-alkyne [3 + 2] cycloaddition proved to be an ideal reaction in very good to excellent yields. 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 DAB-Am-4,8 Core region. The dendritic polymers were characterized by 1H-NMR spectroscopy and IR spectroscopy.

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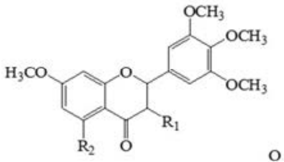
Polyphenol profile from the different tissues of Korean Petasites japonicus (Meowi): Overall contribution to antioxidant activities

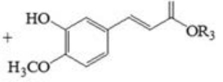
DestaKebedeTaye

경상대학교 화학과

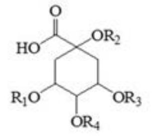
Petasites japonicus, also known locally as Meowi, is ubiquitous in the northern hemisphere where it usually grows in marshy soil, damp forest and alongside rivers and streams. The plant has been used in folk medicine to treat various health ailments including stomach ulcers, headaches, cough, fever, and anxiety. Bioassay investigations indicated that the plant has anticancer and anti-mutagenic effects where polyphenols involvement is highly expected. Despite its various applications, studies focusing on its polyphenol investigations are very scarce. In this study, ten polyphenols were analyzed from the leaf, stem, and roots of Petasites japonicus using LC-ESI-MS/MS method. Components were analyzed according to their [M-H]- ion, MS/MS fragmentation pattern and UV-Vis absorption data along with extensive literature comparison. Structural analysis indicated the presence of three dicaffeoylquinic acid isomers, which are abundant in the genus Petasites. On the other hand, quantification of individual polyphenols was performed using structurally related standards having similar chromophore. The result showed that one of the dicaffeoylquinic acid isomer as a dominant component. The polyphenol extract also showed ranges of antioxidant activities. Validation of the developed LC-ESI-MS/MS method is underway.



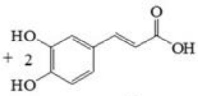
1: $R_1 + R_2 = 2OH$ +



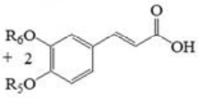
R_3 = glucosyl



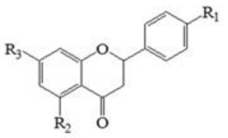
2, 4, 7: $R_1 + R_2 + R_3 + R_4 =$ 2H + 2



8: $R_1 + R_2 + R_3 + R_4 =$ 2H + 2

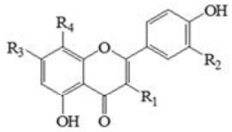


$R_5 + R_6$ = H + hexosyl



3: R_1, R_2 = OH; R_3 = *O*-glucosyl

6: R_1= *O*-glucosyl; R_2 = H; R_3 = OH



5: R_1 = H; R_2 =OH; R_3 = *O*-dihydrogalloylglucosyl;

R_4 = *C*-pentosylglucoside

9: R_1 = OH; R_2, R_4 = H; R_3 = *O*-acetylglucoside

10: R_1, R_4 = H; R_2, R_3 = OCH_3

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Bis-pyrrolidinium Organic Ionic Plastic Crystals

채현호 이민재*

군산대학교 화학과

A series of 1,2-bis[N-(N-methyl(or *1H*)pyrrolidinium)]ethane salts have been synthesized as new organic ionic plastic crystals (OIPCs). Bis-*1H*-pyrrolidinium hexafluorophosphate salt shows multiple solid-solid phase transitions; two distinct heat absorptions at -11 ℃ and 159 ℃. However, its Cl^- and I^- salts do not have any transition. All the bis-(N-methylpyrrolidinium) salts have multiple solid-solid phase transitions even with a asymmetric and highly polarizable bis(trifluoromethylsulfone)imide (Tf_2N) anion (T_{ss} = 38 and 85 ℃, T_m = 207 ℃). Thermal stabilities of the salts were investigated by thermal gravimetric analysis; halide salts are less stable than PF_6 or Tf_2N salts. 1,2-Bis[N-(N-methylpyrrolidinium)]ethane Tf_2N^- show a relatively small entropy of fusion, $\Delta S_f = 27\ \mathrm{J\ mol^{-1}\ K^{-1}}$, which is a close value of Timmermans' definition of plastic crystals ($\Delta S_f = 20\ \mathrm{J\ mol^{-1}\ K^{-1}}$).

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Systemized Functional Group Controls in Polydiacetylenes

한나래 유광호 김민*

충북대학교 화학과

Polydiacetylenes (PDAs), a polymeric system of the diacetylene functional group containing molecules, are very unique micelle type molecular system. These specific vesicles could be polymerized with UV irradiation and ultrasonic treatments in aqueous media. And this photopolymerization of diacetylene forms an array of acetylene-ethylene backbone with delocalized π-electrons. The polymerized vesicle solution with these compounds showed blue to red colorimetric transitions by external stimuli such as temperature, pH, molecular or ion contact, solvent, and etc. Since the color changes of PDAs are detectable by naked eyes, it has been developed effective sensor for variable stimuli.[1-4]

Even though a lot of researches about PDA were reported, the mechanism of the color change in PDA system is not fully investigated in both experimental and theoretical levels. Recently we have designed and synthesized PCDA (pentacosa-10,12-diynoylic acid) derivatives, which have different linker lengths of head group. These series of PCDA derivatives showed different colors (blue, purple, red) at room temperature. The correlation between intramolecular distance and color of PDA will be discussed in this presentation. In addition, we have performed that the functionalization of PCDA molecules with a series of polar or non-polar functional groups. The polarity-controlled PCDA molecules show an elevation of color-changing (blue to red) temperature. We believe that these two experimental finding allow many insights to understand color changing mechanism of PDAs.

References

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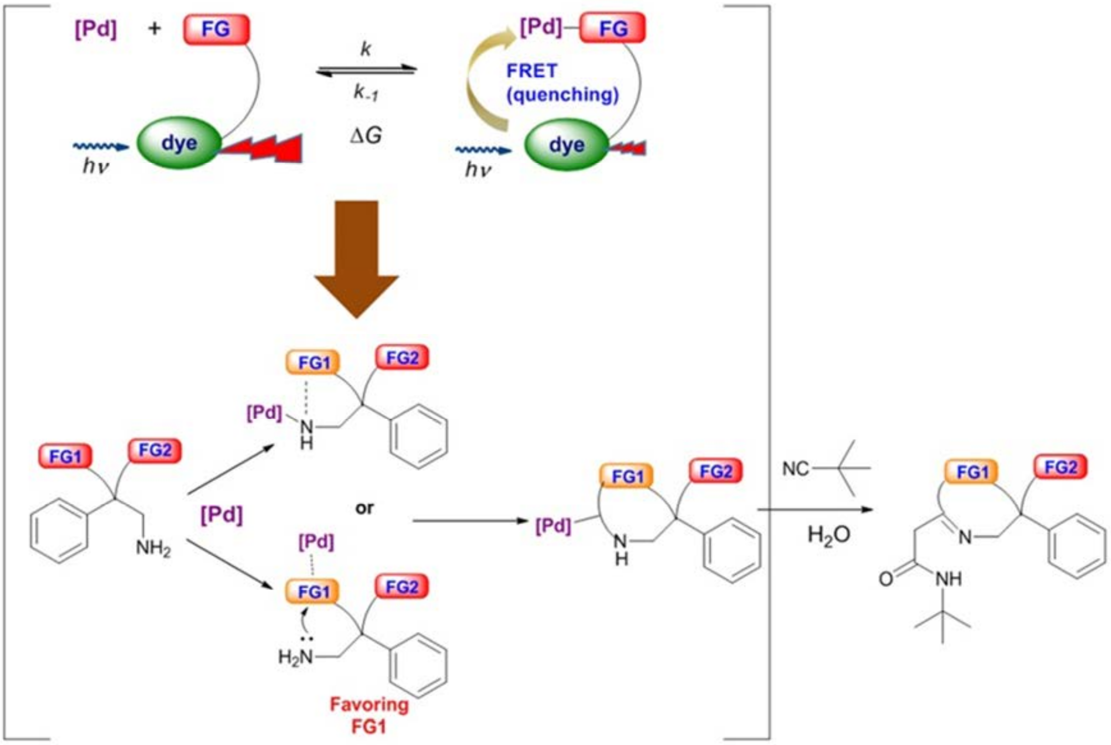
Chemoselective hydroamination reaction guided by the preference of metal catalyst toward carbon-carbon multiple bonds

이지홍 손정훈*

충남대학교 화학과

Transition metal-catalyzed hydroamiation reaction, the direct addition of amino group to carbon-carbon multiple bond such as alkene, alkyne or allene, has been evaluated as an efficient method for synthesis of amine compounds.[1] Although some theoretical studies have given clues for the reaction mechanism, understanding of the detailed hydroamination reaction is still lacking, which causes selectivity issues. Especially, it is hard to predict chemoselectivity of the hydroamination of the substrates possessing multiple functional groups. Furthermore, it is also in dispute whether the catalyst reacts first toward amino group or carbon-carbon multiple bond. As an effort to solving such issues, we employed FRET-based method to determine the functionality preference of metal catalyst.[2] Using this method we established the preference of palladium catalysts toward alkene, alkyne, allene, and amine, and applied it to hydroamination reactions of the substrates containing aminoenyne, aminoallenyne, and aminoallene to achieve chemoselective cyclization. We also presents a cascade process of the palladium-catalyzed hydroamination followed by carbon-carbon bond formation with isocyanide. References1. (a) Müller, T. E.; Hultzsch, K. C.; Yus, M.; Foubelo, F.; Tada, M. Chem. Rev. 2008, 108, 3795. (b) Huang, M. Arndt, K. Gooßen, H. Heydt, L. J. Gooßen, Chem. Rev. 2015, 115, 2596.2. (a) Sohn, J.-H.; Kim, K. H.; Lee, H.-Y.; No, Z. S.; Ihee, H. J. Am. Chem. Soc. 2008, 130, 16506. (b) Kim, K. H.; Ok, T.; Lee, K.; Lee, H.-S.; Chang, K. T.; Ihee, H.; Sohn, J.-H. J. Am. Chem. Soc. 2010, 132, 12027. (c) O. S. Lee, K. H. Kim, J. Kim, K. Kwon, T. Ok, H. Ihee, H. –Y. Lee, J. –H. Sohn, J. Org. Chem. 2013, 78, 8242. (d) Lee, J. H.; Kim, K. Lee, O. S.; Choi, T. –L.; Lee, H. –S.; Ihee, H.; Sohn, J. –H. J. Org. Chem. 2016, 81, 7591.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Bis-piperidinium Organic Ionic Plastic Crystals

채현호 이민재*

군산대학교 화학과

A series of bis-piperidinium salts have been synthesized as new organic ionic plastic crystals (OIPCs). Bis-*1H*-piperidinium hexafluorophosphate salt shows one solid-solid phase transition at 207 ℃, but its Cl^- and I^- salts do not. All the bis-(N-methylpiperidinium) salts have multiple solid-solid phase transitions even with a asymmetric and highly polarizable bis(trifluoromethylsulfone)imide (Tf_2N) anion (T_{ss} = 52 ℃ and 167 ℃, T_m = 227 ℃). Thermal stabilities of the salts were investigated by thermal gravimetric analysis; the halide salts are less stable than PF_6 or Tf_2N salts. 1,2-Bis[N-(N-methylpiperidinium)]ethane Tf_2N^- show a small entropy of fusion, ΔS_f = 31 J mol^{-1} K^{-1}, which is a close value of Timmermans' definition of plastic crystals (ΔS_f = 20 J mol^{-1} K^{-1}).

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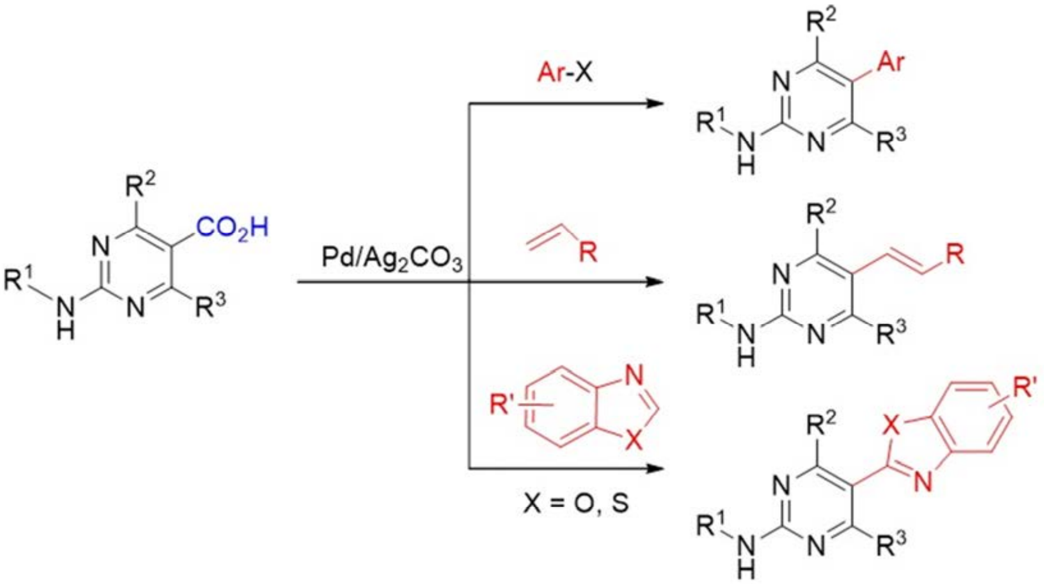
Decarboxylative cross-coupling of 2-aminopyrimindines

LE PHAM NGOC SON 손정훈*

충남대학교 화학과

The 2-aminopyrimidine compounds are embedded as important substructures of many valuable drug candidates or intermediate of drugs, as evidenced by the well-known rosuvastatin (Crestor) and imatinib (Gleevec). They have also been proven to trigger the inhibition of protein kinases or receptors in many development candidates.[1] Despite their biological importance, the synthetic strategy towards these compounds is limited in scope and generality, especially for the rapid generation of a diverse range of such compounds. As an effort to such goals, herein we present palladium-catalyzed decarboxylative carbon-carbon cross-couplings of 2-aminopyrimidine-5-carboxylic acids with arylhalides, olefins, and benzoxazoles (benzothiazoles). Since the 2-aminopyrimidine-5-carboxylic acids can be synthesized in two steps through Biginelli three-component reaction followed by dehydrosulfurative C-N cross-coupling/oxidative dehydrogenation,[2] the decarboxylative cross-coupling could offer facile preparation and diversification of fully substituted 2-aminopyrimidine compounds. References1.(a) Noble, E. M. M.; Endicott, J. A.; Johnson, L. N. Science 2004, 303, 1800. (b) Han, Y. T.; Choi, G. –I.; Son, D.; Kim, N. –J.; Yun, H.; Lee, S.; Chang, D. J.; Hong, H. –S.; Kim, H.; Ha, H. –J.; Kim, Y. –H.; Park, H. –J.; Lee, J.; Suh, Y. –G. J. Med. Chem. 2012, 55, 91202.Phan, N. H. T.; Kim, H.; Shin, H.; Lee, H. –S.; Sohn, J. –H. Org. Lett. 2016, 18, 5154.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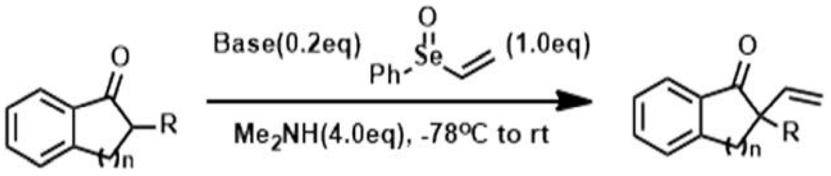
Phenylvinyl selenoxide; A new reagent for one step α-vinylation of ketones

김지헌 이희윤*

KAIST 화학과

Vinyl groups are widely used in organic reactions preparation of such as Cope/Claisen rearrangement, cycloaddition and olefin metathesis. To extend the synthetic utility, α-vinyl ketones have been much desired and the preparation of α-vinyl ketones required ethylene with Pd catalysts or employment of two step process with phenylvinyl sulfoxide or selenoacetaldehyde. Recently, there have been much effort to generation α-vinylation using transition metal catalyst. However, there are some weakness like temperature condition, reaction time and dealing with transition metal. Herein, we present one step process to introduce α-vinyl group to ketones using phenylvinyl selenoxide.Reference1. Derrick L. J. Clive,* Charles G. Russell,' and Suresh Chander Suri J. Org. Chem. Vol. 47, No. 9, 1982 2. R. Tanikaga, H. Sugihara, K. Tanaka, and A. Kaji, Synthesis, 299 (1977) 3. Hans J. Reich,*2S usan Wollowitz, John E. Trend, Flora Chow, and Daniel F. Wendelborn J. Org. Chem., Vol. 43, No. 9, 19784. Yiyang Liu, Scott C. Virgil, Robert H. Grubbs, and Brian M. Stoltz Angew.Chem.Int. Ed. 2015, 54,11800–118035. Jinkun Huang,* Emilio Bunel, and Margaret M. Faul Org. Lett.Vol. 9, No. 21, 2007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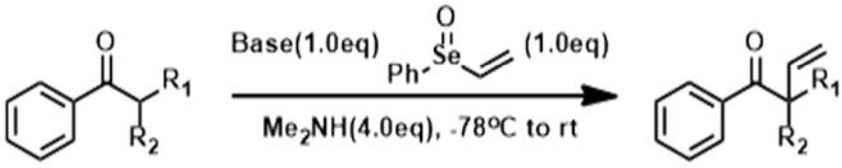
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발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of new photochromic polymer and study of its physical properties

김세미 윤호준[1] 안광현*

경희대학교 응용화학과 [1]경희대학교 화학과

In general, the photochromic material is colored when exposed to ultraviolet light, and returns to its original color upon irradiation with visible light. When such a photochromic material is made of a polymer, various applications such as optical switch, opto-optic devices, and molecular electronic devices become possible.BrBTT was synthesized from BTT, a diarylethene photochromic material as a starting material. BrBTT was used for the synthesis of BTT-Ph-CH_2=CH_2 , which is the basic unit of the polymer through Suzuki reaction. And then the photochromic polymer was prepared using AIBN. The molecular weight is measured to check whether the polymer is produced.And then, The absorption spectra and fluorescence were taken to confirm the photochromic-property of the polymer. The fatigue property of the polymer was also studied.

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UV Irradiation Mediated Palladium Nanoparticle Catalytic System for the Heck and Decarboxylative coupling Reactions

유수빈 김한성 최현철* 이선우*

전남대학교 화학과

Palladium-catalyzed cross coupling reactions have become one of the powerful tools in organic chemistry and been widely used in the preparation of useful building blocks in the organic synthesis fields including material chemistry and pharmaceutical industry. In the coupling reaction with aryl halides, the catalytic activity of palladium is highly dependent on the property of ligands. It was known that electron donating and sterically bulky ligands accelerated the rate of the oxidation step which is the rate determining step in most cross coupling reactions. Therefore, a number of new ligands have been developed and applied in the cross coupling reactions. However, there are some drawbacks that most of them required the multistep synthetic process and it is expensive if some of them are commercially available. To address these issues, we employed Pd-CNT-TiO_2 as a recyclable and high active catalyst, which has received much attention in the metal-catalyzed transformation and cross coupling reactions and a variety of supporting materials for palladium nanoparticle have been developed. For the Heck reaction, 4-iodotoluene and n-butylacrylate as standard substrates were reacted with Et_3N in the presence of Pd-CNT-$TiO_2$2

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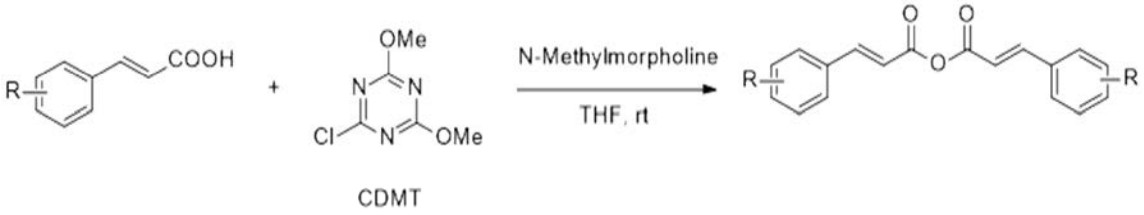
Synthesis of Symmetrical Cinnamic Anhydrides using CDMT as Coupling Reagent at Room temperature

김명진 GABRIELCHARLESEDWINRAJA 이선우*

전남대학교 화학과

A simple and convenient synthetic methodology has been developed for the synthesis of symmetrical alkene anhydrides using cinnamic acids with 2-chloro-4,6-dimethoxy-1,3,5-triazine (CDMT) as coupling reagent and *N*-methylmorpholine (NMM) as base in THF at room temperature. CDMT has been studied well as a coupling reagent for various reactions; here in we report our new methodology for the synthesis symmetrical cinnamic anhydrides. This methodology holds several advantages such as (i) One pot synthesis (ii) simple isolation procedure (iii) mild conditions (iv) by-product of CDMT could be reprocessed back to active CDMT via simple chlorination method. AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)



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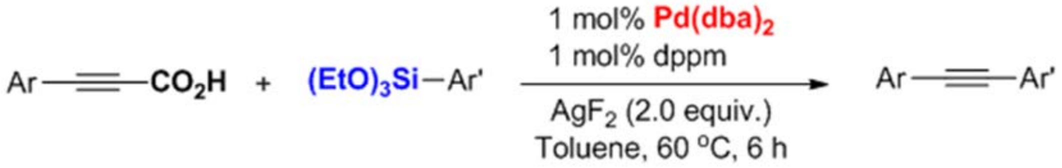
Palladium-Catalyzed Decarboxylative Coupling Reaction of Arylpropiolic Acids Acids with Arylsiloxanes at Mild condition

장지선 이선우*

전남대학교 화학과

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. It 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. 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. And a palladium-catalyzed coupling of terminal alkyne and organosilane was reported by Cheng. However the decarboxyltive coupling reaction of carboxylic acid 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.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)



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Oxidative Decarboxylative Coupling Reactions with Arylpropiolic Acids and Aryl Boronic Acids using a Nickel Catalyst

조은정 이주현 이선우*

전남대학교 화학과

Decarboxylative coupling reactions were generally known for reactions under catalysts such as palladium or copper. As nickel is abundant and much cheaper than palladium, the use of nickel is reasonable. However, a nickel-based catalytic system has not been developed so far. Therefore, we study a decarboxylative coupling reaction between arylpropiolic acids and organoboranes using a nickel catalyst. Herein we report nickel-catalyzed decarboxylative coupling reaction of arylpropiolic acids with aryl boronic acids. When arylpropiolic 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.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)

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Nickel-catalyzed decarboxylative coupling reactions with alkynyl carboxylic acids and aryl iodides

손유정 이선우*

전남대학교 화학과

Decarboxylative coupling reactions are most cases catalyzed by palladium or copper. There are only a few rare examples of nickel catalysts being reported. Recently, we reported nickel-catalyzed decarboxylative coupling reactions of aryl siloxanes or aryl boronic acids. These successes prompted us to develop a nickel-catalyzed decarboxylative coupling reaction with aryl halides. Herein, we report for the first time the nickel-catalyzed decarboxylative coupling of an alkynyl carboxylic acid and aryl iodides. In case of cross-coupling of aryl halide, Ni(COD)$_2$ is the most commonly employed as nickel source. Because Ni(COD)$_2$ is air-sensitive and difficult to handle, we employed the much more stable nickel(II) as a nickel source in the presence of manganese. It is noteworthy that no formation of 1,4-diphenylbutadiyne, which is always produced in palladium- or copper-catalyzed coupling reactions with alkynes, is observed.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)

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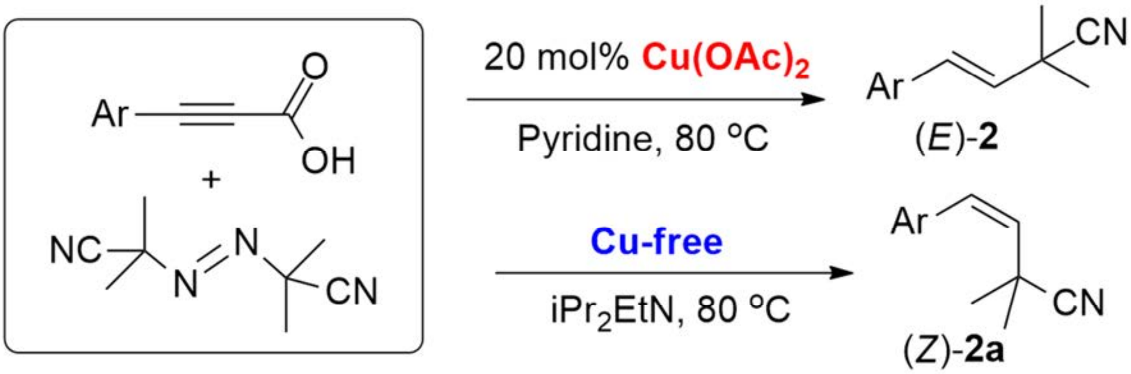
Selective Synthesis of (*E*)- and (*Z*)-Allyl Nitriles via Decarboxylative Reactions of Alkynyl Carboxylic acids with Azobis(isobutyronitrile) (AIBN)

GABRIELCHARLESEDWINRAJA 이선우*

전남대학교 화학과

The nitrile group is one of the most important functional groups in organic synthesis. It is found in natural products and has been introduced into functional materials, pharmaceuticals and other bioactive compounds. Moreover, it plays a key role in the synthesis of functional organic compounds because it is readily converted to other useful functional groups such as amines, amides and carboxylic acids. In particular, the allyl nitrile (or allylcyano) group has been found in bioactive compounds such as the vitamin D receptor, pesticides, and antifungal agents.In our report, Allyl nitriles were synthesized from the reactions of aryl propiolic acids with azobis(isobutyronitrile) (AIBN). In the presence of $Cu(OAc)_2$ as a catalyst, and pyridine as the solvent, the (*E*)-stereoisomer was formed as the major product. This transformation shows good tolerance toward alkoxy, halogen, alcohol, amine, ester and ketone functional groups. When the reaction was conducted with the sterically bulky amine, ethyldiisopropylamine, in the absence of a copper catalyst, the corresponding (*Z*)-stereoisomers were formed preferentially. AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036).


Ar
O
OH
+
NC
N
N
CN
20 mol% Cu(OAc)₂
Pyridine, 80 °C
Ar
CN
(E)-2
Cu-free
iPr₂EtN, 80 °C
Ar
CN
(Z)-2a

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장소: 일산 KINTEX

발표코드: **ORGN.P-284**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Zeolite-Cu Heterogeneous catalyzed decarboxylative cross-coupling reaction of alkynyl carboxylic acid with aryl iodides

박재림 이선우*

전남대학교 화학과

Aryl alkyne moiety is important building block in natural and medical products. Sonogashira type Cu-catalyzed decarboxylative coupling reaction is powerful method to synthesize aryl alkyne moiety. This reaction employed propiolic acid as alkyne source and aryl halides as coupling partner. However, it has disadvantage that diyne is formed through homo-coupling of alkyne source as byproduct. To improve selectivity, we employed a heterogeneous zeolite-Cu catalystic system. This FAU type zeolite Catalyst has frame and hole. Cu remain both inside the hole and frame. Because the size of hole is limited, The chance of homo-coupling between alkyne source is lower than other Cu catalyst. As a result, cross-coupling reaction is predominant, and the reaction has a high selectivity. Herein, we report the zeolite-copper-catalyzed decarboxylative coupling reaction.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)

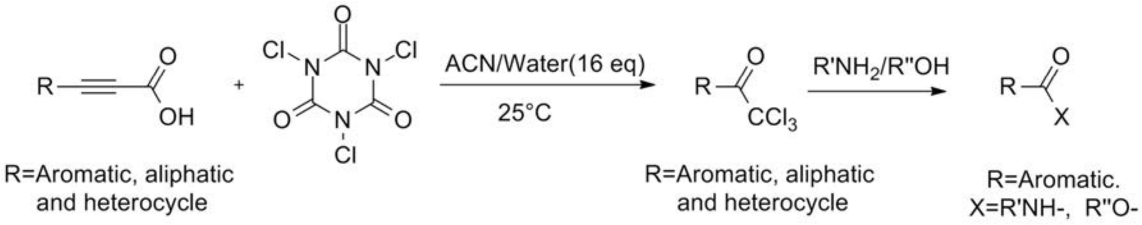
일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-285**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Transition Metal free Decarboxylative oxytrichlorination for Synthesis of 2,2,2-Trichloroacetophenone

JAYARAMAN ARAVINDAN 이선우*

전남대학교 화학과

Recently we developed a transition-metal free decarboxylation reaction for the synthesis of 2,2,2-trichloroacetophenone using alkynyl carboxylic acid and trichloroisocyanuric acid. 2,2,2-trichloroacetophenone are considered to be a suitable alternative for acid chloride under aqueous condition. This is considered to be a novel method for converting the sp carbon of the alkynyl carboxylic acid to a good leaving group. The carbonyl group acts as a Nucleophilic centre; hence various nucleophile like amine and alcohol were reacted in one pot fashion to convert into the corresponding amide and ester.Phenylpropiolic acid was treated with trichloroisocyanuric acid in ACN/water at 23-25°C over a period of 16 h to afford 2,2,2-trichloroacetophenone. This reaction condition tolerated various substituents such as alkyl, halides, nitro, cyano, ketone, and ester functional groups with good yields.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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Palladium Catalyzed Decarboxylative Coupling of Aryl Tosylates with Alkynyl Carboxylic Acids

이주현 이선우*

전남대학교 화학과

The transition metal-catalyzed coupling reactions with aryl halides and nucleophiles have tremendously been developed and widely used in the fields requiring organic synthesis chemistry such as material industry. Aryl triflates and mesylates have been frequently used as pseudo aryl halides. But, they have some drawbacks that the former requires the high cost of triflating agents and the latter shows low activity. The examples of other coupling reactions with aryl tosylates were reported. However, decarboxylative coupling reaction of aryl tosylates has not been developed so far. Compared to aryl halides, aryl tosylates are usually less expensive and more readily available from phenols. Herein, we report a decarboxylative coupling reaction between alkynyl carboxylic acids and aryl tosylates using a palladium catalyst.AcknowledgmentsThis research was supported by a National Research Foundation of Korea (NRF) grant provided by the Korean government (MSIP) (NRF-2014R1A2A1A11050018, NRF-2015R1A4A1041036)

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장소: 일산 KINTEX

발표코드: **ORGN.P-287**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

A highly selective and sensitive turn-on ECL chemodosimeter for hydrazine based on an cyclometalated Ir(III) Complex

김경록 홍종인*

서울대학교 화학부

Hydrazine is an important chemical reagent as a reducing agent or base for industrial processes. Due to the similar properties to water, hydrazine is readily internalized into human body through skin or by inhalation, which then acts as a severe mutagen as well as a neurotoxin to various organs. To date, only few hydrazine-selective chemodosimeters are reported thus a development of highly selective and sensitive sensor to hydrazine is of particular interest.Electrogenerated chemiluminescence(ECL), a luminescent process through sequential electron transfer reactions on the surface of electrode, is a powerful candidate for point-of-care-testing(POCT) due to high sensitivity, simple equipment and good reproducibility. Herein, we developed a turn-on ECL chemodosimeter based on cyclometalated Ir(III) complex for the detection of hydrazine. The probe contains o-Hydroxybenzaldehyde moieties to sense hydrazine in the main ligand. The hydroxyl group activate proximal aldehyde through intramolecular hydrogen bonding, resulting in the effective reaction with hydrazine. Details of synthesis, photophysical and electrochemical properties will be presented.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Electrogenerated Chemiluminescent Sensor Based on Iridium(III) complex for Discriminative Detection of Cysteine over Homocysteine

김태민 홍종인*

서울대학교 화학부

Biological thiols play important roles in living organisms. Cysteine, an essential amino acid, is associated with detoxification, protein synthesis, and metabolism. Selective detection of structurally similar cysteine and homocysteine remains challenging. Although many fluorescent cysteine probes have been developed, they require huge spectroscopic instruments and light sources. Compared to conventional fluorescent techniques, the electrogenerated chemiluminescence (ECL) assay has numerous advantages including high sensitivity, a wide linear response range, and good reproducibility. Herein, we report a new ECL chemosensor based on cyclometalated iridium (III) complex for discriminative detection of cysteine over homocysteine. Probe 1 contains α, β-unsaturated ester (acrylate) moiety in the main ligand, which is a well-known PET quencher. It can react with cysteine selectively by different kinetics of intramolecular conjugate addition-cyclization, enabling phosphorescence enhancement and ECL decrease in the blue-shifted region. We demonstrate the first ECL-based cysteine-selective sensor. Details of synthesis, characterization, and ECL studies will be presented.

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Ir (III) complex-based turn-on ECL sensor for hypochlorite with high selectivity and sensitivity

이하영 홍종인[1,*]

서울대학교 화학과 [1]서울대학교 화학부

Hypochlorite (HOCl), one of the important reactive oxygen species (ROS) in living organisms, plays a vital role in many biological processes. However, excessive accumulations inside human body is proven to cause oxidative damage to tissue and a wide range of diseases, including Parkinson’s disease, atherosclerosis and cancers. Thus, it is necessary to monitor the level of HOCl and therefore, several techniques such as colorimetry and fluorescence have been developed for the detection of HOCl. Still there are some challenges regarding these techniques such as high detection limits and complexity of operation. To overcome these problems, we selected a technic called electrogenerated chemiluminescence (ECL) for detecting hypochlorite due to its high sensitivity, good reproducibility, and simple analytical process.Herein, we designed a novel ECL turn-on chemosensor for hypochlorite based on cyclometalated Ir (III) complex using phenylpyridine as a main ligand and acetylacetone as an ancillary ligand. Oxathiolane group in the main ligand of probe 1 reacts with hypochlorite selectively, inducing fluorescence quenching and ECL turn-on in the red-shifted region. Details of synthesis, photophysical properties and electrochemical studies will be presented.

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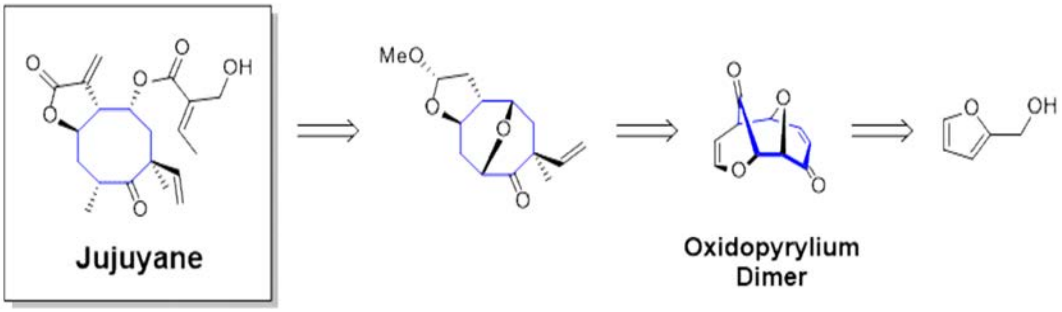
Total Synthesis of Jujuyane

이상현 이희윤*

KAIST 화학과

Oxidopyrylium ylide, which can be prepared from furfuryl alcohol, readily dimerizes in the regio- and stereoselective manner generating doubly bridged carbocycle.[1] Although this dimer is a potential precursor of highly functionalized cyclooctanoids, its application to natural product synthesis has never been reported until today.[2] We accomplished the first total synthesis of Jujuyane, a sesquiterpene lactone isolated from Stevia jujuyansis,[3] utilizing oxidopyrylium dimerization reaction. Stereocenters around a core 8-membered ring structure could be settled by substrate-controlled reactions on the oxa-bridged synthetic intermediate. Subsequent oxa-bridge opening and functional group manipulation completed the total synthesis of Jujuyane.References[1] Hendrickson, J. B.; Farina, J. S. J. Org. Chem., 1980, 45, 3361-3363.[2] Krishna, U. M.; Deodhar, K. D.; Trivedi, G. K.; Mobin, S. M., J. Org. Chem., 2004, 69(3), 967-969 [3] Gil, R. R.; Pacciaroni, A. D. V.; Oberti J. C.; Diaz, J. G.; Herz, W. Phytochemistry, 1992, 31(2), 593-596



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발표코드: **ORGN.P-291**
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발표종류: 포스터, 발표일시: 목 11:00~12:30

Intra-Mitochondrial Biomineralization for New Cancer Therapy

김상필 유자형[1,*] LOGANATHANPALANIKUMAR[2] 최후연[3]

UNIST 분자과학부 [1]UNIST 자연과학부 화학과 [2]UNIST Environmental Scienc [3]UNIST Chemistry

Biomineralization has vital roles for biological process in maintaining tissue homeostasis and cellular function by exploiting inorganic elements. Development of system for controlling biomineralization can be a new tool as potential therapeutic. In this work, we developed mitochondria-targeting biomineralization system by using trialkoxysilane-TPP. Owing to positive charge of TPP, trialkoxysilane-TPP can selectively accumulate inside cancerous mitochondria and accumulation can provide effective condition for forming silica particles via hydrolytic condensation. As that process can be catalyzed by basic condition and accumulation provides effective condition for forming silica particles, silica particles can be formed efficiently inside mitochondria matrix. Formed silica particles depolarized mitochondrial membrane and generate ROS which can be cause of mitochondrial dysfunction, resulting in activation of apoptotic pathways. Thus, our subcellular specific silicification system provides a new insight into the use of intracellular biomineralization for regulating cellular funcations and targeted therapy.

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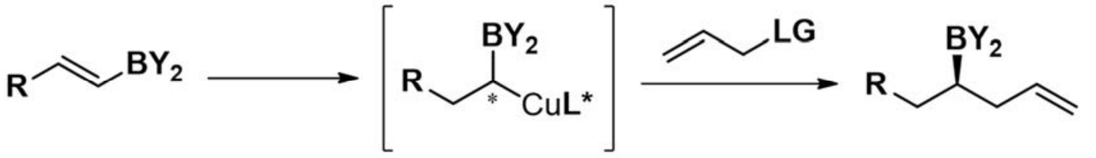
Copper-Catalyzed Enantioselective Hydroallylation: Access to Enantioenriched Homoallylic Boron Compounds

윤재숙* 한정태 장원준

성균관대학교 화학과

Highly enantioselective copper-catalyzed hydroallylation of alkenylborons is achieved. In the presence of CuCl/chiral Walphos catalyst, a variety of alkenylborons provided the borylalkanes in good yield and with excellent enantioselectivity. Pinacolboronates and 1,8-diaminonaphthalene borons with an aryl, heteroaryl, or alkyl substituent were well-tolerated to provide the desired products. To demonstrate the utility of this synthetic method, an efficient synthesis of (S)-massoialactone was presented.



- *up to 97% yield*
- *up to 99 % ee*

BY_2 = Bpin, Bdan

R = aryl, heteroaryl,
H, 1°,2°,3° alkyl

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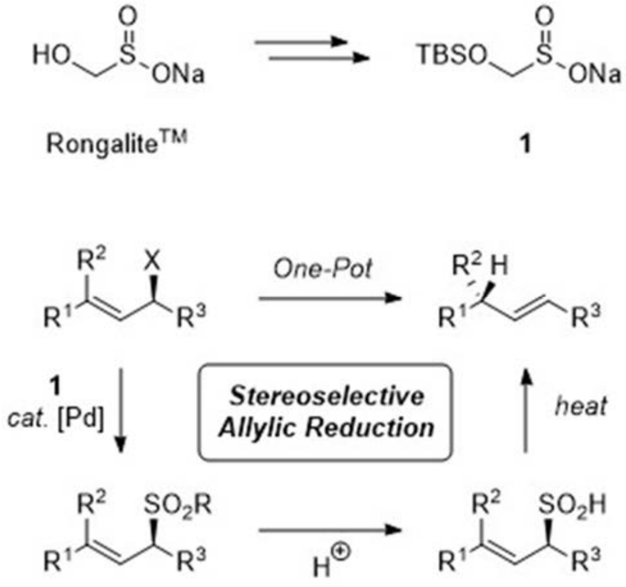
Stereoselective Allylic Reduction Using a Novel Sulfinate

엄현석 이철범[1,*]

서울대학교 자연과학대학/화학부 [1]서울대학교 화학부

The palladium-catalyzed allylic alkylation, also known as the Tsuji-Trost reaction, is a powerful method for the regio- and stereoselective construction of carbon-carbon and carbon-heteroatom bonds.[1] Among numerous variations, the S-allylation has highlighted the synthetic versatility of the process, allowing the allylic C–S bond established by Pd catalysis to be used in the subsequent elaborations. In another line research, our group has recently demonstrated that allylic sulfinic acids, derived from the Diels-Alder reaction of 1-sulfenyl ($TBSOCH_2S$) or sulfonyl ($TBSOCH_2SO_2$) dienes, can be used for the synthesis of unusual cyclohexenes.[2] In an effort to further explore this chemistry in a combined context, we have prepared novel sulfinate reagent **1** from Rongalite®. Described in this poster will be the results of our recent studies on the tandem Tsuji-Trost and retro-ene reactions using sulfinate **1**, in which allylic carbonates are reduced to the alkene products with high regio- and stereoselectivity.[3]

References
(1)B. M. Trost, M. L. Crawley, *Chem. Rev.* **2003**, *103*, 2921.
(2)J. Choi, H. Park, H. J. Yoo, S. Kim, E. J. Sorensen, C. Lee, *J. Am. Chem. Soc.* **2014**, *136*, 9918.
(3)H.-S. Um, Y. Chae, T. An, J. Min, J. Choi, C. Lee, *submitted*.


HO
ONa
Rongalite™
TBSO
ONa
1
One-Pot
1
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Stereoselective Allylic Reduction
heat
SO_2R
$H^{\oplus}$
SO_2H
R^1
R^2
R^3
X
H

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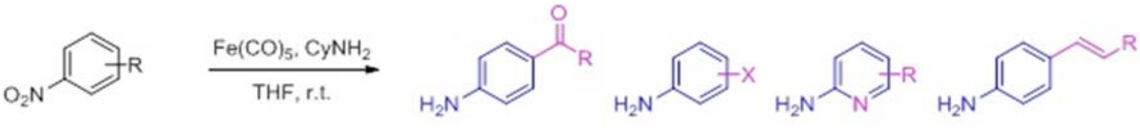
Chemoselective Reduction of Nitroarenes to Anilines Using Iron Carbonyls and Amines as Hydrogen Source

김재형 강은주*

경희대학교 응용화학과

Anilines are widely used as intermediates in the synthesis of dyes, pigments, agrochemicals, and pharmaceuticals. The reductions of nitroarenes to anilines have been carried out under hydrogenation, electron-transfer, electrochemical, and hydride-transfer conditions. But the reduction of more substituted nitroarenes follows byproduct in the presence of functional group can be reduced. For the chemoselective reduction of more substituted nitroarenes, using either hydrazine or formicacid/TEA as a stoichiometric reductant or hydrogen source has been developed.Herein, we use iron pentacarbonyl and cyclohexylamine to reduction more substituted nitroarenes, and report selective nitro reduction product, without byproducts of the other group reduction. It needs stoichiometric iron pentacarbonyl and cyclohexylamine as hydrogen souce, but the reaction is proceeded under mild condition and generate only dicyclohexylurea as byproduct under stoichiometric system mechanism.



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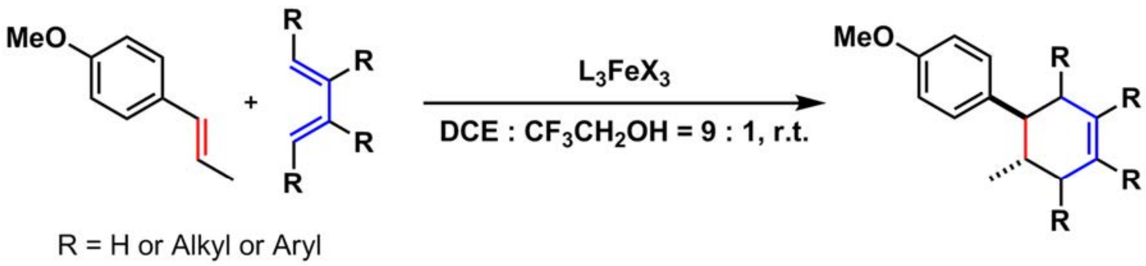
Iron(III)-polypyridyl Complex Catalyzed Radical Cation Cycloaddition Reaction

성은영 강은주*

경희대학교 응용화학과

$Fe(Phen)_3^{3+}$ complex and its derivatives have sufficient oxidizing potential to act as an one-electron oxidant, therby promoting efficient radical cation cycloaddition of electron-rich dienophiles. It is known that photocatalysts or organic catalysts efficiently conduct electron mismatched Diels-Alder reaction or [2+2] cycloaddition as an one-electron oxidant via radical cations of electron-rich olefins. Recent study is going along with Ruthenium(II) or Cr(III) complexes as a photocatalyst and came out into open that chain propagation steps dominate product formation in polar radical cycloaddition mechanism compared to initiation step. We performed this reaction using Fe(III) complexes as effective radical generator although these catalyst can't carry out whole catalytic cycle. Going one step forward, we performed varying ligand of Fe(III) complexes that can result in differential reactivity from established organic catalysts. It can be a facile route to replace rare metals with inexpensive iron to make an effective radical cation cycloaddition reaction.



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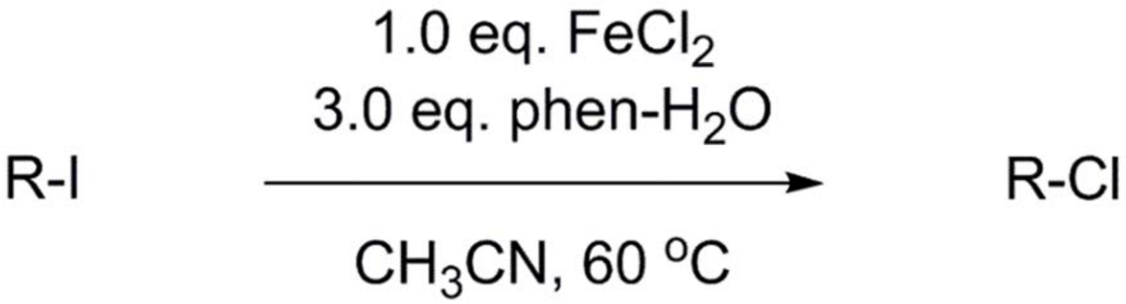
FeCl2-Mediated Nucleophilic Chlorination of Iodoalkanes Accelerated by 1,10-Phenanthroline Ligands

신정하 황준영 강은주*

경희대학교 응용화학과

Over the last years, numerous methods were reported for the chlorination of various organic compounds. They can be divided into nucleophilic chlorination of haloalkanes or alcohol and electrophilic chlorination of alpha substitution of carbonyl compounds. Most of the nucleophilic chlorinations were progressed via oxidative pathway required an oxidant or the reaction condition was slightly harsh with hydrochloric acid as a chloride source. However, we successfully achieved corresponding chlorination products in a single step under mild condition using FeCl2 and 1,10-Phenanthroline system. Furthermore, this reaction system can be applied to primary iodides having various functional groups such as amide, alcohol, acetal, ester and also secondary iodides. We proposed our reaction proceeded by SN2 mechanism in-situ generated Fe(phen)3Cl2 complex and this is the first methodology for ligand-controlled chlorination of iodoalkanes.



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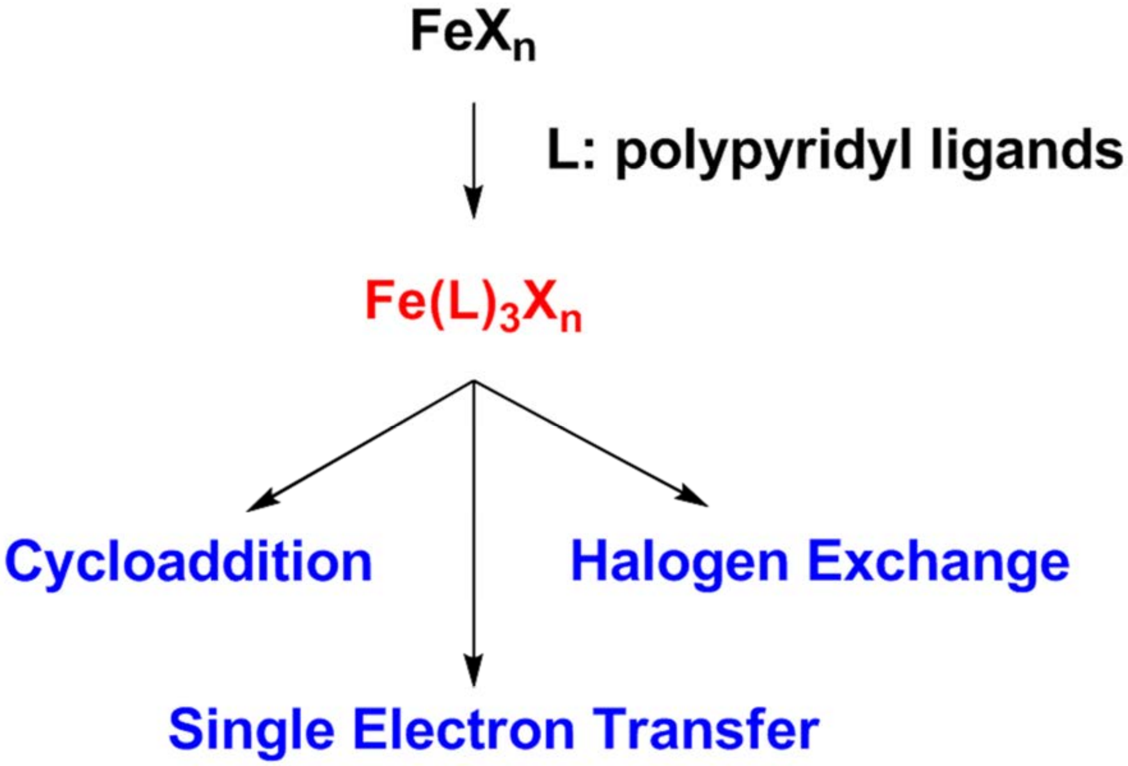
발표종류: 포스터, 발표일시: 목 11:00~12:30

Iron Polypyridyl Complexes: Preperations, Photophysical Properties, and Applications in Organic Reactions Methodology

황준영 성은영 신정하 강은주*

경희대학교 응용화학과

Transition metal complexes (Ru, Ir, Ni, Cu, and Fe) with polypyridyl ligands have been used as important catalysts in single-electron-transfer (SET) organic reactions. Especially, photoredox organic reactions such as radical coupling, asymmetric, cycloaddition, and oxidative/reductive cyclization reactions were developed by using Ru, Ir, Ni, and Cu polypyridyl complexes as photocatalysts. Iron polypyridyl complexes as photosensitizer is not a good candidate for photoinduced electron transfer catalysis due to the short lifetime of the lowest energy excited state. However, Cozzi and Ceroni reported $[Fe(bpy)_3]Br_2$ catalyzed organocatalytic enantioselective alkylation of aldehydes in 2015. Accordingly, in order to develop iron photocatalysis, we investigated photophysical properties of iron polypyridyl complexes: 2,2`-bipyridine, 1,10-phenanthroline, 2,2`:6`,2``-terpyridine, 4,7-dimethyl-1,10-phenanthroline, 3,4,7,8-tetramethyl-1,10-phenanthroline as ligands. Herein, we introduce photophysical properties of iron polypyridyl complexes and applications in radical cross-coupling of oxalate compounds with visible light, chlorination of iodoalkanes, and [2+2] cycloaddition reactions without visible light.


FeX_n
L: polypyridyl ligands
$Fe(L)_3X_n$
Cycloaddition
Halogen Exchange
Single Electron Transfer

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Double N-annulated Isoquinolinium Salt from Allylamine and Internal Alkyne by Rh(III) Catalyst

심수향 한예리 전철호*

연세대학교 화학과

Transition metal catalyzed oxidative annulations through C-H bond activation have attracted much attention for efficient synthesis of heterocyclic compounds. Among the heterocyclic compounds, isoquinolinium cationic moieties are found in many bioactive compounds, pharmaceuticals, and photolumiscent materials. Recently, we developed the synthesis of double N-annulated isoquinolinium salts in one-step synthesis. In the presence of Rh(III), the reaction of primary allylamine and aromatic internal alkyne with Cu(OAc)2 and anion source afforded isoquinolinium salt through C-H activation by Rh(III) catalyst. Various isoquinolinium salts were also prepared from two different alkynes. 2,3-Diphenylpyridine, which is presumed to be an intermediate, was reacted with internal alkyne to afford double N-annulated isoquinolinium salt, too. Fluorescent spectra of isoquinolinium salts with different substituted functional groups were correlated with their wavelengths. Fluorescent spectra shows the emission maxima at λ=430–680 nm, which is blue-to-orange fluorescence emissions depending on the functional group of isoquinolinium salts. Electron donating substituent shows the red shift compared with electron withdrawing substituent. Therefore, we applied this synthetic strategy of isoquinolinium salts to design the compounds with specific wavelength by controlling the substituents.

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장소: 일산 KINTEX
발표코드: **ORGN.P-299**
발표분야: 유기화학
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Highly Dense Immobilization of Dual Functional Polymer onto Silica Nanoparticle and Effect of Chain Length of Functional Group

장지영 박우진 전철호*

연세대학교 화학과

Immobilization of organic compounds onto silica is one of current interests in the material chemistry field. Highly dense functionalization of inorganic materials is important. Alkoxysilane, which is difficult to be functionalized and purified, has been widely used for immobilization of organic compounds. On the other hand, very stable methallylsilane, which can be activated by Sc(OTf)3 catalyst for silica immobilization, can be purified by silica column chromatography. Using silica nanoparticle instead of mesoporous silica enhances loading efficiency on silica surface because its surface area is larger than mesoporous silica. Highly dense immobilization of organic group on silica surface can be achieved by using dual-functional polymer which contains dimethallylsilane moiety as immobilization group and dansyl moiety as functional group. In this report, we report the synthesis of dual functional polymer in which the proportional rate of functional group and immobilization group can be controlled. The effect of chain length can be confirmed by measuring the fluorescence intensity of dansyl functional group. By measuring the fluorescence intensity of dansyl functional group at 510nm, we can observe the effect of carbon chain length connected to the dansyl functional group.

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발표코드: **ORGN.P-300**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Analysis of High energy materials

권국태* 이소정[1] 김승희[2] 김진석*

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

Energetic materials such as TNT, RDX have been studying for a long time. TNT was a major explosive during Worldwar-II and RDX was promising explosive for low cost and high performance. After age of RDX, very few explosives were developed and applicated for the formulation of explosive. It means that it is very difficult to meet conditions which are physicochemical properties, cost, performance and sensitivity issues for next generation of high explosive.As an effort to develop new energetic materials, reaserch about high nitrogen content compound such as azoles was investigated in wide range, because of high heat of formation for N2.Heat of formation is known to be closely related to the energetic properties.Also salt research area is opened for energetic materials, due to their extremely low vapor pressure and relatively high density.Here in, we report synthesis and analysis of triazolium salts for high energy materials.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-301**

발표분야: 유기화학

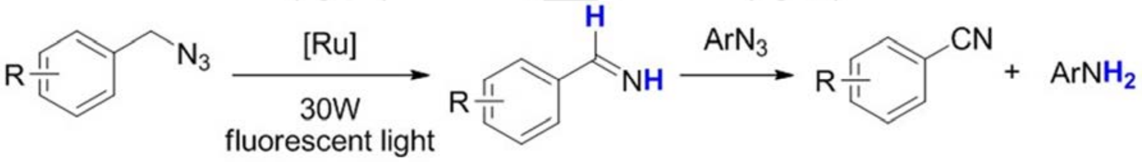
발표종류: 포스터, 발표일시: 목 11:00~12:30

Redox Reaction between Benzyl Azides and Aryl Azides: Concerted Synthesis of Aryl Nitriles and Anilines

김용진 이영호* 박재욱*

POSTECH 화학과

A unique and novel reaction between benzyl azides and aryl azides is described to synthesize aryl nitriles and anilines concurrently, which is catalyzed with a photoactivated diruthenium complex. N-Unsubstituted imines (N–H imines) are generated first from benzyl azides, followed by the hydrogen transfer reaction between N–H imines and aryl azides. A wide range of aryl nitriles and anilines were synthesized under neutral and mild reaction conditions.



- **Catalytic synthesis of aryl nitriles from benzyl azides**
- **Aryl azides acting as mild hydrogen-acceptors with forming anilines**
- **Wide substrate scope**
- **Mild and neutral conditions without additives**

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발표코드: **ORGN.P-302**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

11/9-Helical folding stability of α/β-peptides containing acyclic β-residues

이재연 최수혁*

연세대학교 화학과

In the past two decades, increasing work has been devoted to the study of foldamers that describe any polymer with a strong tendency to adopt specific compact conformation. Mixed helices are distinct and unconventional helical structures, which arise from two types of hydrogen bonds with alternating directions. The α/β-peptide 11/9-helix involves by C=O(i)···H-N(i+3) and C=O(i)···H-N(i-1) hydrogen bonds. Here, we discuss the effect of acyclic β-residue on 11/9-helical folding propensity of α/β-peptides. To test helix stability, we synthesized several penta-peptides and hepta-peptides that contain a β2- or β3-homoalanine. The helical folding stability of these α/β-peptides was analyzed by CD, NMR and IR methods.

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발표분야: 유기화학
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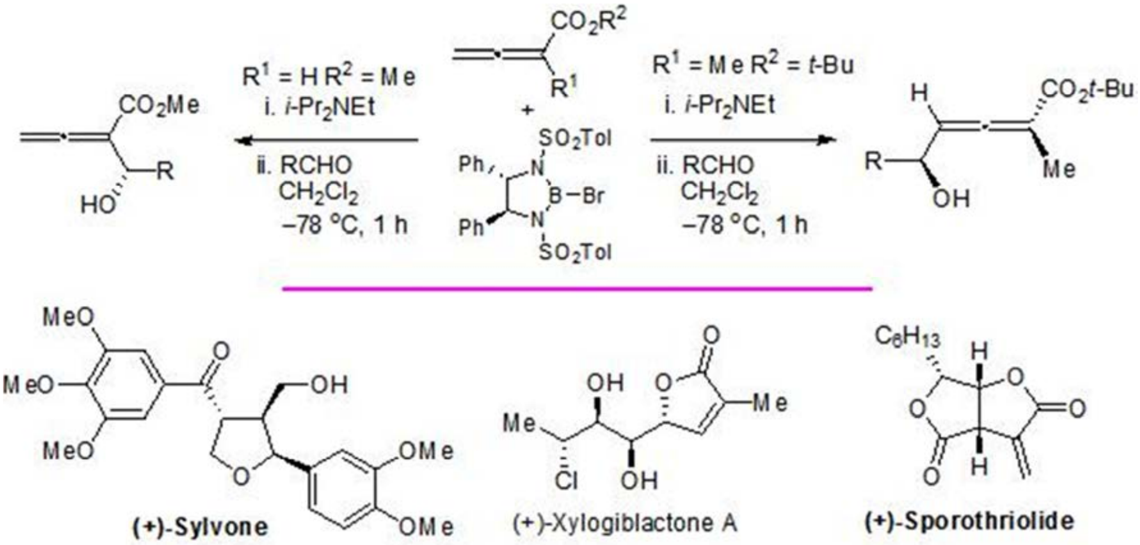
A Highly Efficient Asymmetric Gamma Carbonyl Addition Reaction of Allenoates to Establish Axial and Center Chiraliy

이지은 오창화[1] 박새한샘[1] 박경아[1] 김지민[1,*] 유찬모[*]

성균관대학교 화학과 [1]전남대학교 화학과

Recently, we have disclosed a new aldol method of the allenoate process in forming 2-hydroxy allenolate in high levels of enantioselectivity. For this method the reactin exclusively dictates a regioselectivity starting from methyl allenoate as shown below scheme. Efficient synthesis of a furanolignan (+)-sylvone can be demonstrated their synthetic applicability. As part of our continous investigations utilizing allenoates as versatile substrates for asymmetric carbonyl additions, we establish stereospecific formation of gamma-addition adduct from 1-alkyl allenoates to construct axial and center chiralities during the reaction, which allows in good yields and excellent stereoselectivities. Reaction usually produced only single regio- and stereisomer. We would like to present herein scope and limitation of the reaction and its synthetic applications to natural products.



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장소: 일산 KINTEX
발표코드: **ORGN.P-304**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

An Optimized and Efficient Synthetic Strategy to Prepare Arylnaphthalene Lactone Natural Products

김태정 김경민[1] 강기성[2] 함정엽*

한국과학기술연구원(KIST) 천연물연구소 [1]강릉원주대학교 화학신소재학과 [2]가천대학교 글로벌캠퍼스 한의학과

Arylnaphthalene lactone natural products are plant-derived lignan compounds and have a wide range of biological properties; including anticancer, antiplatelet, antiviral, piscicidal, phosphodiest-erase inhibition, 5-lipooxygenase inhibition, HIV reverse transcriptase inhibition, and antibacterial activities. Furthermore, the unique and simple structure of arylnaphthalene lactones can be used as a template for lead compounds in the development of new drugs derived from natural products.Since their chemical structure was first reported in the 1960's, numerous synthetic strategies to efficiently prepare these natural lignin compounds have been developed, including the tandem reaction of 2-alkynylbenzonitrile, Pd-catalyzed [2+2+2] cocyclization of arynes and diynes, the ring expansion of benzocyclobutenones, the intramolecular dehydro (Pummerer)Diels-Alder reaction, and sequential Horner-Emmons-Claisen condensation. However, previous methods are limited to obtain arylnaphthalene lactone derivatives having basic sensitive functional groups on aryl moiety.Herein, we report a highly efficient synthetic method including Hauser-Kraus annulation of cyanophthalides and Suzuki-Miyaura cross-coupling reaction for the synthesis of arylnaphthalene lactone natural products using cyanophthalides as the starting material. Resultingly, we have successfully synthesized various biologically active arylnaphthalene lactone natural products, such as diphyllin, justicidin A, cilinaphthalide B, taiwanin E, chinensinaphthol, taiwanin E methyl ether, chinensinaphthol methyl ether, justicidin C, and justicidin D.

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장소: 일산 KINTEX
발표코드: **ORGN.P-305**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structural photophysical property relationship study about Indolizine fluorescent core skeleton

최상기 김현기 김은하*

아주대학교 분자과학기술학과

Indolizine is an N-bridgehead bicyclic heterocycle aromatic compound having 10 electrons. Due to its unique chemical structure, many indolizines, which have optical properties and fluorescence properties, have been investigated for their suitability as dyes for dye sensitized solar cell (DSSC) or organic light emitting devices(OLEDs). On the other hand, indolizine is well known pharmacophore and have been found to manifest a various biological activity such as anti-tumor, anti-bacterial, anti-HIV, anti-oxidizing and anti-inflammatory activity. Collectively, indolizine based fluorescent compound may have better chance to specifically interact with biological system. Therefore, we believe the study of structure and photophysical property relationship about indolizine can boost up the speed for discovery of versatile fluorescent bioprobes against multiple different bio-markers. Herein, we want to present systematic study of structure photophysical property relationship about indolizine, focusing on modification site at C-1, C-3 and C-7 position.

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발표코드: **ORGN.P-306**
발표분야: 유기화학
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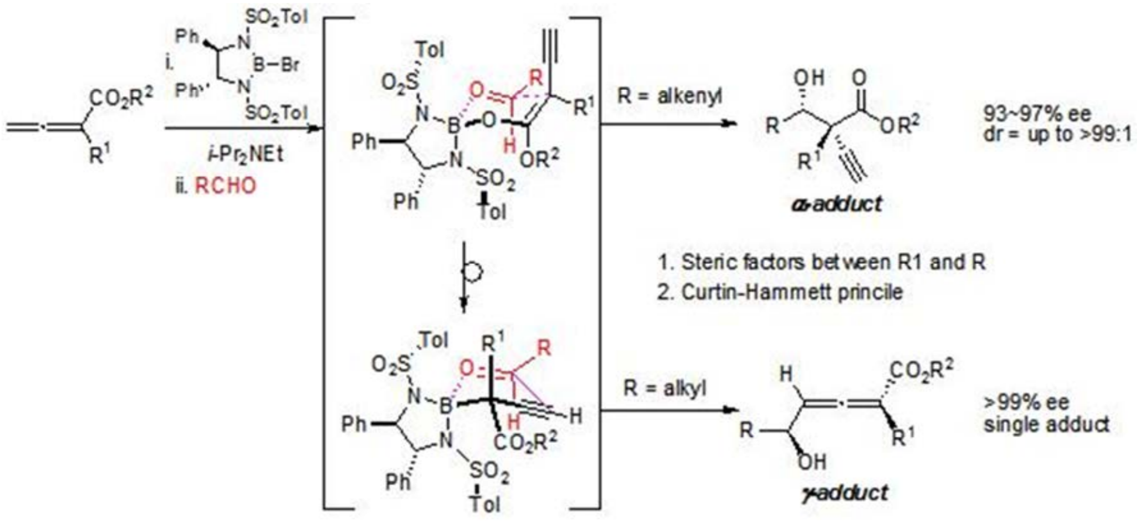
Controlling Factors of Alpha vs Gamma Asymmetric Addition Routes of Allenoates via O-Boron and C-Boron Migration

오창화 정희중 이지은[1] 임태영 유찬모[1,*] 김지민[*]

전남대학교 화학과 [1]성균관대학교 화학과

The discovery of efficient asymmetric methods to achieve the synthesis of enantiomerically pure compounds is of considerable interest in organic chemistry. In light of widespread advances in asymmetric methods, aldol reactions of carbonyl functionalities using chiral auxiliaries or catalysts led to significant developments in the area of asymmetric synthesis. Although there have been many reports regarding the enhancement of chemical processes for practical use, the scope of aldol reactions is still limited to simple systems. As part of our investigations utilizing allenoates as versatile substrates for asymmetric carbonyl additions, we present herein our investigations to find control elements to regulate selective formation of alpha adduct or gamma adducts from the reaction of allenoates with aldehydes depending on substrate geometry as shown in following scheme, which allows in good yields with high levels of stereoselectivity. We will present mainly mechanistic evidences for regio- and stereoselectivity for unprecedented aldol processes of 1-alkyl allenoates and methods of structural elucidation of the products.


CO2R2
R1
i.
Ph
SO2Tol
N
B–Br
N
SO2Tol
i-Pr2NEt
ii. RCHO
Tol
O2S
N
B
O
O
R
H
R1
OR2
Ph
N
SO2
Tol
R = alkenyl
OH
O
R
OR2
R1
α-adduct
93~97% ee
dr = up to >99:1
1. Steric factors between R1 and R
2. Curtin-Hammett princile
R1
R
O
H
H
CO2R2
R = alkyl
H
CO2R2
R
R1
OH
γ-adduct
>99% ee
single adduct

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발표분야: 유기화학
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Three-component synthesis of unsymmetrical diarylalkynes via thermo-controlled sequential Sonogashira reactions

노태섭 김태정[1] 박영태[1] 전상일 함정엽[1,*]

강릉원주대학교 화학과 [1]한국과학기술연구원(KIST) 천연물연구소

The reaction between terminal alkynes and aryl and vinyl halides in the presence of palladium/copper catalysts is known as Sonogashira-Hagihara cross-coupling (Sonogashira reaction), and is one of the most powerful synthetic methods available for the straightforward construction of C(sp)–C(sp^2) bonds. This method has been used to prepare biologically active small molecules, natural products, and engineering materials, and numerous reports have highlighted the utility of this coupling strategy. Furthermore, methods for the preparation of terminal alkynes from aldehydes, vicinal-dihaloalkenes, and geminal-dihaloalkanes have been developed. However, terminal alkynes are costly and cumbersome materials, have low molecular weights and boiling points as well as, a short shelf-life (unstable storage), and are generally difficult to handle. These issues hinder the widespread use of terminal alkynes as Sonogashira coupling partners for aryl or vinyl halides.Herein, we will be described the three-component one-pot synthesis of unsymmetrical diarylalkynes from potassium ethynyltrifluoroborate and two different reactive aryl halides via thermo-controlled sequential Sonogashira reactions

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발표분야: 유기화학
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Synthesis and properties of S1P derivatives with thiol groups at the terminal

박지혜 홍인석*

공주대학교 화학과

Biologically active lipids serve as signaling molecules in human and animal diseases. Among biological active lipids, S1P is secreted in the blood for wound healing, and functions to prevent cells from dying due to stress. As S1P such as a biomarker becomes important, various attempts have been made to detect S1P in blood. In this study, we synthesized S1P derivatives with terminal thiol moiety which can bind to antigen-forming proteins, and confirmed the possibility that they serve as an epitope by ELISA method.

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발표분야: 유기화학
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Highly sensitive ratiometric detection of heparin and its oversulfated chondroitin sulfate contaminant by fluorescent peptidyl probe

Mehta Pramod Kumar 이건형[1,*]

인하대학교 화학화공융합학과 [1]인하대학교 화학과

The selective and sensitive detection of heparin, an anticoagulant in clinics as well as its contaminant oversulfated chondroitin sulfate (OSCS) is of great importance. We first reported a ratiometric sensing method for heparin as well as OSCS contaminants in heparin using a fluorescent peptidyl probe (Pep1, pyrene-GSRKR) and heparin-digestive enzyme. Pep1 exhibited a highly sensitive ratiometric response to nanomolar concentration of heparin in aqueous solution over a wide pH range (2~11) and showed highly selective ratiometric response to heparin among biological competitors such as hyaluronic acid and chondroitin sulfate. Pep1 showed a linear ratiometric response to nanomolar concentrations of heparin in aqueous solutions and in human serum samples. The detection limit for heparin was calculated to be 2.46 nM (R2=0.99) in aqueous solutions, 2.98 nM (R2=0.98) in 1% serum samples, and 3.43 nM (R2=0.99) in 5% serum samples. Pep1 was applied to detect the contaminated OSCS in heparin with heparinase I, II, and III, respectively. The ratiometric sensing method using Pep1 and heparinase II was highly sensitive, fast, and efficient for the detection of OSCS contaminant in heparin. Pep1 with heparinase II could detect as low as 0.0001% (w/w) of OSCS in heparin by a ratiometric response.

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Synthesis and Photochromic Reaction of Merocyanine-sulfonate Photoacid

최고은 신은주*

순천대학교 화학과

Sulfonate-functionalized merocyanine acts as a photoacid. On irradiation of visible light, it can reversibly change large magnitude of proton concentration. The applications of this type of photoacid in controlling proton transfer in chemical, material and biological processes have been reported over the past few years. Sulfonate-functionalized merocyanine photoacid (MEH) undergoes a cyclization reaction under visible light to form a protonated spiropyran (SPH), which is highly acidic. Protonated spiropyran (SPH) releases a proton to form a spiropyran. Therefore, protonated spiropyran as a relatively strong acid is expected to be applicable to various acid-catalyzed chemical reactions. In acidic media, spiropyran associate with proton to form SPH, which revert to MEH, thermally. In this study, we report here that sulfonate-functionalized merocyanine photoacids have been synthesized and characterized by spectroscopic methods. In addition, reversible photochromic reactions of merocyanine photoacids have been investigated.

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Spiropyran-Isoquinoline Dyad as Metal Cation Sensor

고용민 신은주*

순천대학교 화학과

Spiropyran(SP) is one of the promising families of photochromic compounds with respect to external stimuli such as light, thermal, protons, and metal ions. They undergo reversible photoreaction between a closed spiropyran (SP) form that is nearly colorless and an open merocyanine (MC) form that is intensely colored. The neutral spiropyran form cannot act as a chelating ligand for metal cations. The negatively charged phenolic oxygen in the zwitterionic open merocyanine form, which is produced from spiropyran on UV irradiation, efficiently binds with protons and metal ions. Spiropyran-isoquinoline dyad with isoquinoline ring incorporated into spiropyran is expected to be very efficient chelating ligand because both the negatively charged phenolic oxygen and isoquinoline nitrogen may bind cooperatively with protons and metal ions. Therefore, spiropyran-isoquinoline dyad is expected to be excellent light-controlled fluorometric ion sensing system. In this study, a dyad composed of spiropyran and isoquinoline has been prepared and its metal cation-sensing ability has been examined.

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Tuning of the Selectivity of Fluorescent Peptidyl Bioprobe Using Aggregation Induced Emission for Heavy Metal Ions by Buffering Agents in 100% Aqueous Solutions

Neupane Lok Nath 이건형*

인하대학교 화학과

Smart fluorescent probes of which the detection of specific target molecules can be controlled are attracting remarkable interest. A fluorescent peptidyl bioprobe (1) was rationally synthesized by conjugating tetraphenylethylene, an aggregation -in duced emission (AIE) fluorophore with a peptide receptor (AspHis) that acted as hard and intermediate bases. The selective detection of 1 for specific metal ion in 100% aqueous solutions was controlled by the buffering agents with the chelate effect without the change of pH. In distilled water and phosphate buffered aqueous solution at neutral pH, 1 exhibited a selective Off-On response to a soft metal ion, Hg2+ among test metal ions by 100-fold enhancement of the emission at 470 nm. 1 showed a selective Off-On response (180-fold enhancement) to a hard metal ion, Al3+ ions among test metal ions in Tris buffered aqueous solution at neutral pH and Hexamine (hexamethyle netetramine) buffered aqueous solution at acidic pH. The detection limit of 0.46 ppb for Hg2+ and 2.26 ppb for Al3+ in each condition was lower than the maximum allowable level of the metal ions in drinking water by EPA. This research helps to understand how buffering agents participate in the complex formation and aggregation of fluorescent probes using an AIE process for the selective detection of specific metal ions in aqueous solutions.

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Rhodamine-Spiropyran Dyad for Fe3+ detection

김빛나 신은주*

순천대학교 화학과

Rhodamine derivatives have always received high-level attention because of their excellent photostability, suitable photophysical properties, water-solubility, long absorption and emission wavelengths elongated to the visible region, large absorption coefficient and high fluorescence quantum yield. Spiropyran is one of the most widely studied classes of photoswitchable compounds, undergoing reversible structural transformation between a colourless spiropyran form and a coloured merocyanine form upon light, heat or chemical stimulus, which has been shown to exhibit extremely sensitive absorption and colour changes in the visible range. Heavy and transition metal ions have drawn intense attention due to these metals' crucial roles in many environmental and biological processes. Among the metals, iron is the physiologically most abundant and versatile metal in biological systems. It is required of many enzymatic reactions, for example, oxygen uptake, oxygen metabolism, electron transfer, and transcriptional regulation. However, abnormal levels of Fe3+ could cause anemia and breathing problems, certain cancers, dysfunction of certain organs (heart, kidneys, pancreas, and liver), and even neurodegenerative diseases (Parkinson's disease and Alzheimer's disease). Therefore, the simple and fast detection and separation of iron ions are very desirable. For the detection of Fe3+, fluorescent sensors are especially attractive due to their advantages such as high sensitivity, noninvasiveness, and convenience. In this work, rhodamine-spiropyran has been prepared and investigated its ability as a Fe3+ sensor.

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Hydroarylation reaction of styrene with phenol using various mixed catalysts

김빛나 고용민[1] 신은주[*] 안호근[2] 정민철[2]

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Catalytic Hydroarylation reation of styrene with phenol is one of the current interesting and useful reaction to construct a new C-C bond. Hydroarylation reaction of styrene with phenol in the presence of catalyst usually 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. These reactions are usually assisted by either protic acid or Lewis acid. However, these methods have several limitations like the use of stoichiometric amount of Lewis acids, drastic reaction conditions (i.e. high temperature, longer reaction time etc.), lower selectivity, over alkylation products and large amount of salt and waste formation. Thus, identification of an efficient mixed catalytic system for hydroarylation of alkenes remains an intriguing challenge. In this work, hydroarylation of styrene with phenol was studied using various mixed catalyst in mild condition.

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A Study on the Synthesis of Triptycene-*tris*(1,4-benzoquinone)

김준영 류영준 권지언[1] 안병관[*] 박수영[1,*]

가톨릭대학교 화학과 [1]서울대학교 재료공학부

1,4-Benzoquinones (*para*-benzoquinones) are an important class of molecules, which serve as valuable building blocks for the development of new opto-electronic, pharmaceutical and biological materials. In this study, triptycene *tris*(1,4-benzoquinone) (TI-3BQ), in which three 1,4-benzoquinone units are linked three-dimensionally in space, was prepared via various synthetic routes including Diels-Alder and oxidative demethylation reactions. The factors affecting the synthetic yields and the optimal conditions were investigated and discussed in detail.

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Synthesis of diamine compounds with 8-Aza-bicyclo [3.2.1] octan-3-onyl or Saccharide derivatives

배송미 이언진* 정대일 한정태[1]

동아대학교 화학과 [1]영동대학교 뷰티케어과

Tropane alkaloids are a class of bicyclic [3.2.1] alkaloids and some tropane alkaloids have pharmacological properties, which can act as anticholinergics or stimulants. Cocaine and atropine, most widely known tropane alkaloids, all share the same tropane core structure. Cyclic sugars especially in naturally occurring molecules contain furanoses and pyranoses. Glucose and fructose are found naturally in many fruits and some vegetables and are part of a wide variety of metabolic pathways across species. Moreover, saccharide derivatives are reported to possess antiviral activity with low side effects. Our group have been interested in utilizing this unique characteristics of the pyranose scaffold to develop a bioactive drug while reducing undesired side effects. Generally, 8-azabicyclo[3.2.1]octan-3-ones can be obtained by the reaction of diamines(2,3-diaminopyridine or 3,4-diaminotoluene), 2,5-dimethoxy-tetrahydrofuran, and 1,3-acetonedicarboxylic acid. Pyranosyl derivatives can be obtained by the treatment of diamines(1,6-diaminohexane or 1,12-diaminododecane) and pyranoses (glucose, mannose, or galactose) in anhydrous methanol.

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Synthesis novel structure DPP for preventing fluorescence quenching

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서울대학교 공과대학 재료공학부 [1]서울대학교 재료공학부 [2]서울대학교 재료공학과

Diketopyrrolopyrrole(DPP) dyes are adopted on various application, such as photoconversion film and OLED due to their good optical properties and chemical stabilities. When DPP dyes dried and becomes solid state, DPP forms aggregation causing fluorescent quenching. Fluorescent quenching decrease fluorescence intensity therefore dye must be designed to minimize aggregation. In this study three kinds of DPP derivatives were synthesized. Synthesized dyes contained long alkyl chain on 2, 5 position. This alkyl chain can make DPP molecule bulky and this bulky chain can weaken molecule interaction and minimize aggregation. Synthesis DPP dye's spectral properties were examined by UV-Vis spectroscopy and PL spectroscopy. Consequently three synthesis dyes show reinforce in fluorescence intensity comparing with existing DPP dyes.

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Stimuli-responsive dendrimers with 1,3,5-triazacyclohexane core for the delivery of nucleic acid therapeutics

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동아대학교 화학과 [1]영동대학교 뷰티케어과

RNA interference (RNAi) is a disease gene disruption strategy with enormous potential. RNAi can be achieved by delivering small interfering RNA (siRNA) to target tissues effectively and safely. The choice of the delivery vehicle is a major tackle in RNAi. Dendrimers, which are useful candidates for the delivery vehicle, have properties such as highly defined structure, multivalency, and molecular uniformity and are biologically active under the influence of peripheral groups and generation numbers. In addition, a number of studies have suggested that the flexibility of the core play an important role in the biological activity. Although dendrimers promise many advantageous properties such as extremely low polydispersity and molecular homogeneity, it also causes toxicity problems due to large molecular weight and large surface area. Therefore, biodegradable dendrimers that break down into biologically harmless small molecules after successful delivery of siRNAs are highly needed.In this study, stimuli-responsive 1,3,5-triazacyclohexane are synthesized from amino acids such as cysteine, glycine and serine with biodegradable branches. Incorporating biodegradable linker in the branch is expected to decrease the cytotoxicity as well as possible side effects.

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A study on the synthesis of 1H-1,5-benzodiazepines with acetone equivalents and oximes

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동아대학교 화학과 [1]영동대학교 뷰티케어과

Benzodiazepines are interesting compounds, which can improve the effectiveness of the neurotransmitter, GABA and therefore benzodiazepine derivatives are used as sedatives or anticonvulsants. Industrial applications of benzodiazepines are found in photography used as dyes for acrylic fibers. Despite their wide range of pharmaceutical, industrial and synthetic applications, the synthesis of 1H-1,5-benzodiazepines has received relatively little attention.Herein, we now report the synthesis of 1H-1,5-benzodiazepine derivatives with heteroaromatic ketones and oximes. The direct reaction of diamines and oximes were found not to occur. We have found that dichloramine-T can used to efficiently convert oximes to the corresponding carbonyl compounds. Use of dichloramine-T and new deoximating reagent to synthesize various benzodiazepines are summarized.

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Synthesis of N-(11H-indeno[1,2-b]quinoxalin-11-ylidenes) and Spiro[imidazolidine-4,11'-indeno[1,2-b]quinoxalin-hydantoins

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동아대학교 화학과 [1]영동대학교 뷰티케어과

Indenoquinoxaline derivatives in organic synthesis are an important class of nitrogen-containing heterocycles and are useful building blocks found in a wide range of biologically active compounds. Moreover, carbonyl group of indeno[1,2-b]quinoxalin-11-ones can further be modified to pharmacologically important functional groups such as hydantoin ring or Schiff base. Hydantoin is found in medically important compounds such as the anticonvulsants, phenytoin and fosphenytoin, which are used to treat seizure disorders. Schiff bases have been reported to possess a wide range of medicinal and pharmacological activities such as anticonvulsants, anti-inflammatory agents, analgesics and antimicrobial agents. In this study, a series of indeno[1,2-b]quinoxalin-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]quinoxalin-11-one derivatives were further reacted to form hydantoins and Schiff base moieties. 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]quinoxalin-11-one derivatives.

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Hypoxia response drug delivery system

김지선 서진호 정태호 구세영 김수빈 김종승*

고려대학교 화학과

An azobenzene scaffold serves as both a fluorescence quencher and nitrogen mustard deactivator in a mitochondrial targeting unit bearing theranostic drug delivery system (DDS). The DDS exhibited a tissue selectivity for tumors with aggressive phenotypes, and the efficient in vitro and in vivo azoreduction under hypoxia conditions resulted in bright fluorescence at the tumor site as well as the in situ activation of the prodrug. In vivo therapeutic experiments demonstrated a significant reduction in tumor growth versus number of controls and ex vivo tissue analysis confirmed tissue normalization with strongly reduced angiogenic markers and suppressed cell proliferation. Mechanistic insight of the DDS's mode of action was gained by gene and protein expression experiments, aided by a proteomic analysis, revealing the circumvention of cellular drug resistance pathways as well as the normalization of Slit-Robo signaling, and the involvement of granzyme-triggered mitochondria-mediated apoptosis. Overall the combined high sensitivity and synthetic ease as well as excellent therapeutic response suggests a revival of the azobenzene class of hypoxia activated drugs, especially applied to theranostics, is warranted.

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Facile synthetic routes for furo[3,2-c]coumarin derivatives as potent tyrosinase inhibitors

김재현 이구연* 황운상

강원대학교 생명건강공학과

Tyrosinase is a multifunctional, glycosylated, and copper-containing oxidase, which catalyzes the first two steps in mammalian melanogenesis and is responsible for enzymatic browning reactions in damaged fruits during post-harvest handling and processing. These phenomena have encouraged researchers to seek new potent tyrosinase inhibitors for use in foods and cosmetics. Many compounds have been reported to inhibit tyrosinase activity but furo[3,2-c]coumarins have not been reported. The most potent coumarin was found to be 2-methyl-1-phenyl-11H-benzo[h]furo[3,2-c]coumarin which induces 72% inhibition at 5 mM concentration and is highly effective when compared to ascorbic acid, one of the best tyrosinase inhibitors known so far. In this poster, we will report the facile synthetic methods for the preparation of furo[3,2-c]coumarin derivatives and their tyrosinase inhibition assay.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (No. 2015H1C1A1035955).

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Development of a new synthetic strategy of aurone derivatives as potent tyrosinase inhibitors

김재현 이구연* 황운상

강원대학교 생명건강공학과

Tyrosinase is a multifunctional copper-containing enzyme, playing a key role in melanin biosynthesis by catalyzing the oxidation of phenol to o-quinone observed in the early stage of various browning phenomena in nature, such as melanization in animals and browning in plants. Tyrosinase inhibitors can therefore be clinically useful for the treatment of some dermatological disorders associated with melanin hyperpigmentation. The most potent aurone was found to be (Z)-2-(4-methoxybenzylidene)benzofuran-3(2H)-one which induces 78% inhibition at 5 mM concentration and is highly effective when compared to ascorbic acid, one of the best tyrosinase inhibitors known so far. In this study, naturally occurring aurones was investigated and showed their tyrosinase inhibition effect.This work was supported by the Human Resource Training Program for Regional Innovation and Creativity through the Ministry of Education and National Research Foundation of Korea (No. 2015H1C1A1035955).

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Oxazolidine-based dual optical probe for galactosidase

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A dual optical probe based on a fused oxazolidinoindocyanine moiety was prepared for detection of b-galactosidase in the biological condition. The probe displayed both a dramatic colorless-to-red optical change and a fluorescence turn-on response in the visible region, exhibiting a high sensitivity for b-galactosidase with a very low limit of detection (LOD = 0.071 U/L) in neutral PBS buffer. References: 1. G. P. Dimri, X. Lee, G. Basile, M. Acosta, G. Scott, C. Roskelley, Proc. Natl. Acad. Sci. U.S.A. 1995, 92, 9363-9367.2. V. Bassaneze, A. A. Miyakawa, J. E. Krieger, Anal Biochem. 2008, 372, 198-203.3. B.Y. Lee, J.A. Han, J.S. Im, A. Morrone, K. Johung, E.C. Goodwin, Aging Cell. 2006, 5, 187-195.4. S-Y. Na, H-J. Kim. Dyes Pigm. 2016, 134, 526-530.

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Pyrone-derived ratiometric fluorescent probe for galactosidase with a dramatic fluorescence change

서현석 김해조[1,*]

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b-Galactosidase (b-Gal) is an enzyme to catalyze the hydrolysis of a glycosidic bond of b-galactopyranoside within a carbohydrate such as lactose, ganglioside GM1, and lactoceramides. Commonly, it is employed as a reporter marker to monitor gene expression of lacZ.1,2,3. A simple pyrone-derived fluorescent probe was designed for fluorescent detection of b-galactosidase. Upon reaction with the enzyme, the fluorescent probe underwent a dramatic ratiometric fluorescence change capable of quantitative detection of b-galactosidase.References: 1. C. L. Dobson, A. J. Warren, R. Pannell, A. Forster, T. H. Rabbitts, EMBO J. 2000, 19, 843–851.2. G. P. Dimri, X. Lee, G. Basile, M. Acosta, G. Scott, C. Roskelley, E. E. Medrano, M. Linskens, I. Rubelj, O. Pereira-Smith, Proc. Natl. Acad. Sci. U.S.A. 1995, 92, 9363–7.3. J. P. Horwitz, J. Chua, R. J. Curby, A. J. Tomson, M. A. Da Rooge, B. E. Fisher, J. Mauricio, I. Klundt, J Mater Chem B Mater Biol Med. 1964, 7, 574-575.

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Targeted tumor surveillance: guideline recommendation for next-generation biotinylated diagnostics

구세영 박근영 심인섭 신원섭 김종승*

고려대학교 화학과

Precision cancer medicine initiative relies on the validated tumor-associated features provided by genomic studies to classify the patient subtypes depending upon plausible health risk, diagnosis and treatment response, with the ulti-mate goal of conveying the most efficient treatment modality to the patients. In this regard, considerable challenges incorporate how to advance and/or improve and execute the new as well as the previous targeted therapeutic strate-gies. Although prominent progress has been made recently, yet the modifications in the existing paradigms are simi-larly expected to enhance the remedial outcomes in order to realize the tumor associated features. In this respects, we have developed a biotin-based cancer imaging conjugates to investigate the prominent role of hydrophilicity on their efficient cellular uptake process. The conjugate 5 with logPoct ~ 1 exhibited preferential cell membrane uptake through SMVT proteins under PKC-mediation in vitro. In spite of biotin aided cancer targeting, particular hydrophilicity as-sumes a critical part in general cell uptake process and are specially facilitated by utilizing intracellular ATPs. We demonstrate the importance of such regulation in biotinylated imaging and targeted strategies are an interesting and promising perspective to be considered under the fate of precision medicine.

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Triphenylamine core based hole transporting materials for red phosphorescence based OLEDs

김수현 **POTHUPITIYA GAMAGESUDESH JAYASHANTHA** 채규윤*

원광대학교 화학과

In this work, we have designed, synthesized and characterized four novel hole transporting materials (HTMs) namely, 4a, 4b, 5a and 5b based on triphenylamine central core for OLED application. Which were synthesized with moderate yields by using well known Suzuki coupling reaction. All materials except HTM 4a showed stable decomposition temperature over 410 oCat 5% weight reduction. HTM 4b and 5b were exhibited higher glass transition temperature of 216 oC and 181 oC, respectively. Red phosphorescence based devices were fabricated in order to understand the device efficiencies and NPB based device was used as reference for our current study. The device structure consist of HTM 5a as hole transporting material showed excellent maximum current and power efficiencies of 30.3 cd/A and 34.7 lm/W when compare to other synthesized HTMs. The above noticed values were exhibited similar characteristics with NPB based reference device.

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Selective Formation of Distyrenated Phenol in the Reaction of Styrene with Phenol

고용민 김빛나 신은주[*] 안호근[1] 정민철[1]

순천대학교 화학과 [1]순천대학교 화학공학과

Addition reaction of styrene to phenol in the presence of catalyst gave the mixture of styrenated phenols, which are composed of o-mono-styrenated phenols (o-MSP) and p-mono-styrenated phenols (p-MSP), o,o-di-styrenated phenols (o,o-DSP) and o,p-di-styrenated phenols (o,p-DSP), and o,o,p-tri-styrenated phenol (TSP). Styrenated phenols are sort of sterically hindered phenols. Technical mixture of these styrenated phenols including MSP, DSP, and TSP has been commonly applied for industrial materials such as rubber or plastic stabilizer, antioxidant, and nonionic surfactant, etc. Among these styrenated phenols, o,o-DSP containing ortho bulky substituents is expected to show high performance as antioxidants. Therefore, DSP should be most effective as rubber and plastic stabilizers. Therefore, mixture of styrenated phenols with higher content of DSP is more desirable to be used as antioxidant. DSP is not only more hindered phenol, but also better compatibility with polymers than MSP. However, the preparation of o,o-DSP as the sole product is highly difficult because other styrenated phenol derivatives of o-MSP, p-MSP, o,p-DSP, and TSP are formed along with o,o-DSP. We have investigated the hydroarylation reaction of styrene with phenol to find the optimal catalyst to get high selectivity to DSP under mild reaction conditions.

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Beta-galactosidase triggered in vivo imaging agent

김지현 신진우 선우경 손수빈 김형석 김종승*

고려대학교 화학과

Development of targeted, selective, and noninvasive fluorescent probes for in vivo visualization of tumor-associated overexpressed enzymes are highly anticipated for cancer diagnosis and therapy. Herein, we developed a noninvasive fluorescent probe (DCDHF-bgal) for the sensitive detection, and in vivo visualization of b-galactosidase in hepatocyte HepG2 cells and its xenograft model. As a model system for in vivo targeted imaging, DCDHF-bgal possessing galactose unit selectively target hepatocyte and monitor the b-galactosidase activity with deep tissue penetration, and low background interference. DCDHF-bgal was activated by intracellular b-galactosidases as the driving force for the release of NIR fluorophore, thereby exhibiting ratiometric optical response. Initial fluorescence emission measured at 615 nm was changed to fluorescence at 665 nm upon activation of DCDHF-bgal with b-galactosidase. Ratiometric fluorescence detection of b-galactosidase was also observed in hepatocellular carcinoma cells and tumor xenograft. The noninvasive in vivo optical imaging facilitated by targeted and enzyme-activated imaging agent would be useful in various biomedical and diagnostic applications.

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Carbazole central core based small molecular hole transporting materials for OLEDs

주미라 채규윤* 김수현 양기훈

원광대학교 화학과

A series of carbazole based hole transporting materials namely, 7a, 7b and 7c were designed and synthesized by using Buchwald-Hartwig amination reaction with reasonable yield over 66 %. HTMs 7a and 7b showed higher decomposition temperatures of 400 and 380 oC without any crystalline features and also revealed good solubility in most of the organic solvents. Among the designed HTMs, HTM 7a based red phosphorescence device was exhibited similar device performance with NPB based reference device. The current and power efficiencies were 28.2 cd/A and 26.5 lm/W for HTM 7a based device, which was higher than that of HTM 7b and 7c. HTM 7c showed poor device characteristics due to its higher hole injection barrier (0.44 eV).

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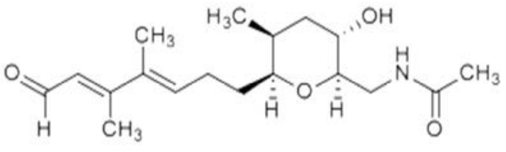
Synthesis of Tetrahydropyran Core Parts in Brevisamide and Spliceostatins E

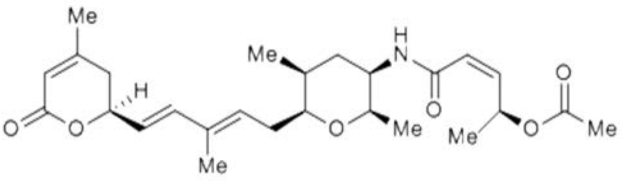
강한영* 정소리

충북대학교 화학과

Because tetrahydropyrans (THPs) are commonly found in a variety of natural products, synthesis of the six-membered oxacycles in stereoselective fashion have attracted a lot of attention. We have been interested in substituted tetrahydropyrans in connection with our endeavors towards to the total synthesis of THP-containing natural products. Our interests have been focused on Brevisamide (1) and Spliceostatin E (2) specifically, due to their relatively simple structures. Cyclization to the oxacyclic structures have been an important subject for the natural products having THPs with an array of many stereogenic centers. We have examined mainly two synthetic strategies, that is, those employing either epoxide opening or iodoetherification to prepare THPs. Our efforts to study the stereoselective cyclization to substituted THPs will be presented.



Brevisamide (**1**)



Spliceostatin E (**2**)

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Coordination-driven self-assembly using phenanthrene-based pyridyl donors and Ru(II) *p*-cymene acceptors

김동환 **SINGH NEM** 지기환*

울산대학교 화학과

In the past two decades, coordination-driven self-assembly has emerged as an efficient method for constructing metalla-supramolecules of numerous shapes, size and topologies, which have shown promising applications such as molecular recognition, separation, catalysis and encapsulation of various guests. In this work we have demostrated the use of a phenanthrene-derived pyridyl donors in spontaneous formation of new metalla-supramolecules by its coordination-driven self-assembly with various Ru(II) p-cymene acceptors. The resulting supramolecular complexes have been characterized by various spectroscopic and single crystal X-ray diffraction analyses. The poster will address a detail comprehensive account of the mentioned work.

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Synthesis of molecular rectangles based on triazole-derived donors and arene ruthenium acceptors via coordination-driven self-assembly

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울산대학교 화학과

In recent years, coordination-driven self-assembly has become dominant method for constructing functionalized metallosupramolecular architectures with promising biological, electronic, and photophysical properties. In addition, these systems have been used in molecular recognition, drug delivery and catalysis. Hence, molecules with enhanced properties for use in metallosupramolecular systems would be desirable to the research community. The coordination-driven self-assembly of new triazole based donors with various arene ruthenium acceptors have resulted in formation of new metallosupramolecular architectures. All the new metallosupramolecules have been characterized by elemental analysis, ^{1}H NMR, ^{13}C NMR and mass spectrometry. The poster will address a detail comprehensive account of the mentioned work.

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Encapsulation studies of iridium(III)-derived self-assembled trigonal cage

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울산대학교 화학과

Confined space inside the self-assembled coordination cages is being successfully used in various challenging applications such as encapsulation and stabilization of insoluble and reactive molecules, recognition of reactive intermediates, catalysis and so on. Recently some coordination cages self-assembled using square planer 90° Pd and Pt acceptor were shown to demonstrate these exciting applications. In this work, the iridium(iii) cornered self-assembled metallacage was encapsulated with up to three planer platinum(II) and palladium(II) acetylacetonate complexes. All the new complexes were characterized by various spectroscopic analysis and single crystal X-ray diffraction. The poster will present a detail comprehensive account of the mentioned work.

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Rational design of a photo-crosslinking BODIPY for in situ protein labeling

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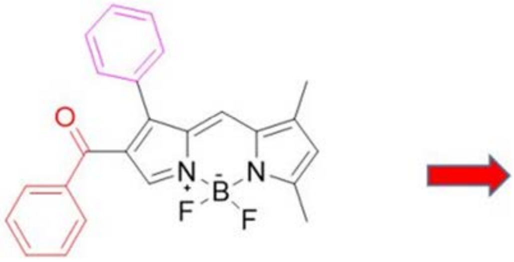
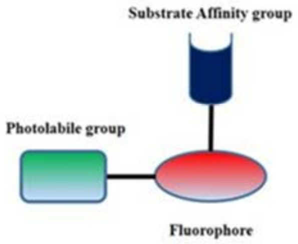
Photo-crosslinking agents have emerged as critical tools to investigate protein-protein interactions (PPI) in complex proteome, but there are few photocrosslinkers available at the moment. Here, we report the first rational design of a photo-crosslinking BODIPY fluorophore (pcBD) and its biological application for biomolecule labeling in a spatiotemporally controlled manner. As a photosensitizing functional motif, the aryl ketone group was incorporated into BODIPY fluorophore, and series of proteins were labeled by pcBD compounds upon UV irradiations. The main success of this design is, this works better than benzophenone, also it has BODIPY fluorophore so can be used as fluorescent tag. This BODIPY-benzophenone conjugate system has the capability to attach BODIPY fluorophore at any kind of target protein depending on the spatial vicinity via photo-affinity labelling. We have designed photo-crosslinking fluorophore with linkers that can easily be utilized to introduce substrate affinity group. The substrate affinity group can direct the probe localization into the specific organelle in which target protein reside. PPIs of target protein can be easily visualized upon photo-irradiation, and we are under investigation of series of targets playing role in reactive oxygen species (ROS) signaling and autophagy pathway.



pcBD1a - c



Schematic representation of the BODIPY-benzophenone conjugate Probes for substrate affinity labelling

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Facile synthesis of gamma backbone of peptide nucleic acid

김초롱 홍인석*

공주대학교 화학과

Many modifications to the aminoethylglycine backbone have been studied to improve the properties of peptide nulcleic acid. In particular, the introduction of a chiral environment at the gamma position has been reported to increase or decrease the binding affinity to DNA, and the demand for gamma PNA backbone is increasing. However, in the case of traditional synthetic methods, the gamma backbone was synthesized by reductive amination using chiral aldehyde derivatives and glycine esters. In this case, the yield is low and it is difficult to synthesize a large scale. In this study, we report the facile synthesis of gamma PNA backbone through Mitsunobu reaction and confirmed the possibility of large scale synthesis.

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Synthesis and Application of a New Type of Benzyne Precursor

권용주 전영교 김원석[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

Benzyne is highly strained and reactive alkyne. Generally, benzyne is derived from an aromatic ring by removal of two ortho substituents. A lot of attempts to make benzyne intermediate have been reported because of its great activity and usefulness. Nowadays, various applications using silylaryl triflate in the presence of fluoride source has been reported. Herein, a new type of benzyne precursor without using fluoride anion source is designed, synthesized and evaluated. It is capable of highly reactive benzyne intermediate induced by 1,3-silyl group migration on the aryl moiety. Moreover, in order to make various benzyne moieties, boron was introduced on the aryl moiety by C-H borylation. Then the boron reagent was used for Suzuki-Miyaura coupling. To install methoxy group on the aryl moiety, oxidation followed by methylation of the boron reagent was attempted. Finally, to understand a mechanism, crossover experiment employing benzyne precursors having TBS or TIPS group respectively, has been investigated.

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Synthesis and high throughput screening of fluorescent library for detecting bio-molecules

홍성철 HAQUE MD MAMUNUL[1] 이준석[2,*]

과학기술연합대학원대학교(UST) 생물화학 [1]한국과학기술연구원(KIST) Biomolecular Recogni [2]한국과학기술연구원(KIST) 분자인지연구센터

Fluorophores have been studied to develop novel bio-molecule sensors in the cell. Their environmental-sensitive properties (e.g. Bathochromic or hypsochromic shift, Increase or decrease intensity) provide various type of probe, but few recognition domains limits scope of target molecule. To overcome this limitation, “diversity-oriented fluorescence library approaches” (DOFLA) has emerged to identify novel bio-sensor scaffold for various biological targets. In DOFLA, combinatorial library of fluorephores, which potentially change their fluorescence color or intensity, were screened against biologically relevant molecules, and it is even possible to discover novel probes without knowledges of molecular recognition mode for target molecule. Here, we prepared fluorescent library based on 1-dimethylaminonaphthalene-5-sulfonyl chloride (dansyl chloride), 2-(2’-hydroxyphenyl)-benzimidazole (HBI) and fluorescein fluorophore. We collected fluorescence emission responses of the diversity-oriented fluorescence library compounds to various bio-molecules, including amino acids, steroids, reactive oxygen species (ROS), metal ions, and etc. Based on our fluorescence response profile, we found several lead compounds for bio-molecule sensors. Our results demonstrated the potential application of this library in biosensors, bio-imaging and target indicators.

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A Fluorescent Probe for Specific Detection of Hydrogen Sulfide Based on a Familiar ESIPT Fluorophore

정예린 윤주영[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

Hydrogen sulfide (H_2S) which has been known as a rotten eggs smell gas has been identified as the third gasotransmitter following nitric oxide (NO) and carbon monoxide (CO). In quite a long time, hydrogen sulfide was considered to be an absolute toxic gas and environmental pollutant. However, this view was modified as H_2S was first observed to present as a neuromodulator in the brain in 1996. As a matter of fact, hydrogen sulfide is also the smallest member among reactive sulfur species (RSS), making major contributions to the function of mammalian tissues. For example, the imbalance of hydrogen sulfide in living system may be harmful to peripheral and central nervous systems, leading to Down's syndrome, Huntington's, Parkinson's, and Alzheimer's diseases. Accompanied by the critical biological function of hydrogen sulfide, the chemical detection method of hydrogen sulfide in vivo has attracted considerable attention. Consequently, sustained research efforts have been devoted to the development of efficient strategies for detection of hydrogen sulfide. In contrast to the electro-chemical methods, gas chromatography, the fluorescent probes based on small molecules have been more attractive owing to its simplicity, high sensitivity, noninvasiveness, and real-time detection in living systems.9 Recently, a large number of fluorescent probes for H_2S have been developed. However, most of these probes are based on fluorophores which may suffer from small Stokes shift and/or undergo aggregation caused quenching (ACQ) in aqueous or physiological media. Hydrogen sulfide (H_2S) is a signaling gasotransmitter which fulfills various roles in modulating the functions of different systems. In this study, we developed a "turn-on" fluorescent probe for H_2S based on a familiar ESIPT fluorophore bearing AIE characteristic. The probe exhibited 80-fold fluorescent enhancement upon addition of H_2S with large Stokes shift. Furthermore, the probe has been successfully applied to detecting H_2S in HeLa cells.

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Development of A Novel Synthetic Route for Benzo[a]carbazoles

전지예 박진재 천철홍*

고려대학교 화학과

Carbazole and its derivatives have been found in a number of biologically important natural products and pharmaceuticals. In addition, they have been utilized as useful scaffolds in materials sciences since they display unique optical and electric properties. Thus, the development of a novel synthetic protocol to access carbazole and its derivatives and a number of carbazole derivatives have been prepared. Among the various carbazole derivatives, aryl- and heteroaryl-annulated carbazoles have received considerable attention due to their interesting biological and pharmacological activities. Thus, many methods for synthesis the aryl-annulated carbazoles have been developed over the past decades. However, most of previous methods have often required multistep sequences in the preparation of aryl-annulated carbazoles and/or the preparation of starting materials. Thus, it is highly desired to develop a new synthetic route for the synthesis of benzo[a]carbazoles in a step-economical manner.We recently developed synthetic protocols for the synthesis of 2-substituted indole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and aldehydes via intramolecular imino-Stetter reaction using cyanide as the catalyst.1 As a continuing effect to develop a novel method for the synthesis of 2,3-disubstituted indole derivatives using this protocol, we further attempted to develop a new method for the synthesis of benzo[a]carbazole derivatives based on this protocol. 2-Arylindole derivatives bearing a β-ketone moiety at the 3-position were prepared from the aldimines derived from 2-aminobenzylideneacetophenones and aromatic aldehydes via cyanide-catalyzed intramolecular imino-Stetter reaction. Subsequent intramolecular Friedel-Crafts reactions of the resulting 2-arylindole derivatives afforded benzo[a]carbazole derivatives. In this poster presentation, we will disclose our new approach for synthesis the benzo[a]carbazoles from the aldimines via cyanide-catalyzed imino-Stetter reaction followed by intramolecular Friedel-Crafts reaction.

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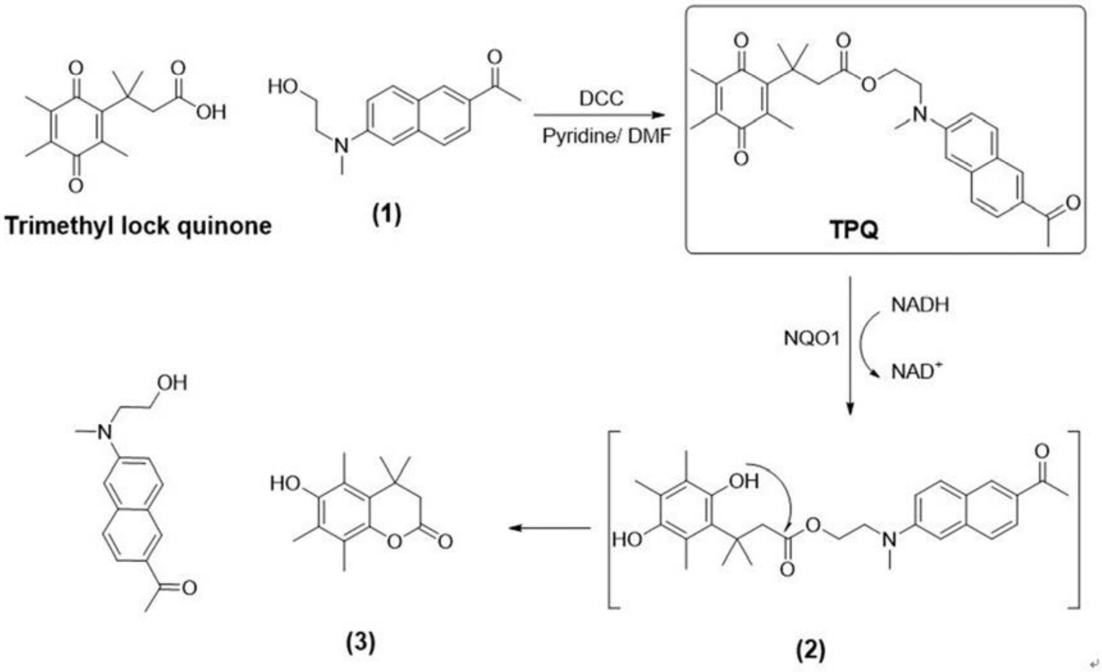
Development of New Two-Photon Fluorescent Probe that Detects Human NAD(P)H:Quinone Oxidoreductase (hNQO1) for Tumor Cell Imaging

권나현 김환명[1,*] 윤주영[2,*]

이화여자대학교 화학나노과학과 [1]아주대학교 화학과/에너지시스템학과 [2]이화여자대학교 화학·나노과학과

Oxidase and reductase related enzymes have attractive recent interest because of their high correlation with cancers. hNQO1 (human NAD(P)H:quinone oxidoreductase, EC 1.6.99.2) is a crucial reductase that is widely distributed and ubiquitously present in all cellular environments including the cytosol, Golgi complex, nucleus, mitochondria, membrane and endoplasmic reticulum, as well as in extracellular components. Utilizing either NADH or NADPH as cofactors, hNQO1 promotes reduction of quinones, quinone epoxides and aromatic nitro compounds. Importantly, the expression level of hNQO1 is much higher in cancer tissues compared to normal tissues. Because of its high resolution and sensitivity, fluorescent imaging has attracted great attention in fields related to biomedicine. In contrast to typical one-photon light fluorescent probes, those that utilize two-photon light (TP) have many advantageous features that expand biological imaging and clinical applications. The following reasoning was employed to design TPQ, a new TP probe, for detection of hNQO1. The 3-methyl-3-(2,4,5-trimethyl-3,6-dioxocyclohexa-1,4-dien-1-yl)butanoic acid (trimethyl lock quinone (tlq)) moiety has been used frequently in the design of prodrugs. Our strategy for the design of the new fluorescence probe for hNQO1 also relies on the tlq moiety. Reduction of TPQ promoted by hNQO1 and NADH gives hydroquinone 2, which undergoes rapid cleavage of the ester moiety with concomitant formation of lactone 3 the reporter fluorophore 1.


Trimethyl lock quinone
(1)
DCC
Pyridine/ DMF
TPQ
NQO1
NADH
NAD⁺
(2)
(3)

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Enantioselective Synthesis of Cyclic β-Arylamines via Chiral Phosphoric Acid-catalyzed Asymmetric Reductive Amination of β-Tetralones

박도영 천철홍*

고려대학교 화학과

Although chiral phosphoric acid-catalyzed asymmetric reduction of ketimines have been widely utilized in the synthesis of chiral amines, most of the previous examples have been limited to the synthesis of acyclic chiral amines via enantioselective reduction of ketimines derived from acyclic ketones, and there have been no previous reports on the enantioselective synthesis of chiral cyclic amines via chiral phosphoric acid-catalyzed asymmetric reductive amination of cyclic ketones. Based on the biological and pharmacological importance of chiral cyclic amines and the lack of the protocols to access these important building blocks, our group has initiated a program for the development of a new method for the enantioselective synthesis of chiral cyclic amines via chiral phosphoric acid-catalyzed asymmetric reductive amination of cyclic ketones. When β-tetralones and aniline derivative were subjected to asymmetric reductive amination with Hantzsch ester as an organic hydride source in the presence of chiral phosphoric acid, the desired cyclic β-arylamines were obtained in good yields and good to high enantioselectivities. In this poster presentation, we will describe the first example of the synthesis of chiral cyclic amines via chiral phosphoric acid-catalyzed asymmetric reductive amination of β-tetralones with aniline derivatives using Hantzsch ester as an organic hydride source.

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발표분야: 유기화학
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Application of perylene dyes for low dielectric hybrid-type black matrices

황태규 김재필* 이우성[1] 노정우[2] 이재문[3] 우성윤[3]

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Organic dyes with low dielectric constant have recently been suggested as a replacement for Cr/CrOx or carbon black in developing black matrices with low dielectric constants for liquid crystal displays. However, due to a spectral property of the dyes which generally shows narrow absorption range, black matrix based on dyes needs to be fabricated by material mixture method. In this study, hybrid-type black matrices were fabricated with various blend ratios of dyes and carbon black to fully absorb visible light and maintain low dielectric constants. The dyes were designed and synthesized based on the perylene moiety (perylenediimide and perylenetetracarboxylic bisbenzimidazole) to overcome non-uniform surfaces caused by dyes of different moieties. Additionally, each dye was designed to have different absorption range, which was affected by its conjugation length and donating ability of bay position substituents, to prevent light leaking. Evaluations of the optical and thermal properties and solubility of the dyes were conducted to confirm its applicability on the black matrix. Dye-type black matrices were also fabricated using two perylene based dyes for comparison with hybrid-type black matrices. The dye-type films had an advantage of small dielectric constants, but their spectral properties were not satisfactory. On the other hand, the hybrid-type films blocked the whole visible light effectively, showed high thermal stability and had good optical and electrical properties. Furthermore, the film roughness was significantly improved compared to that found in previous research by applying the synthesized dyes.

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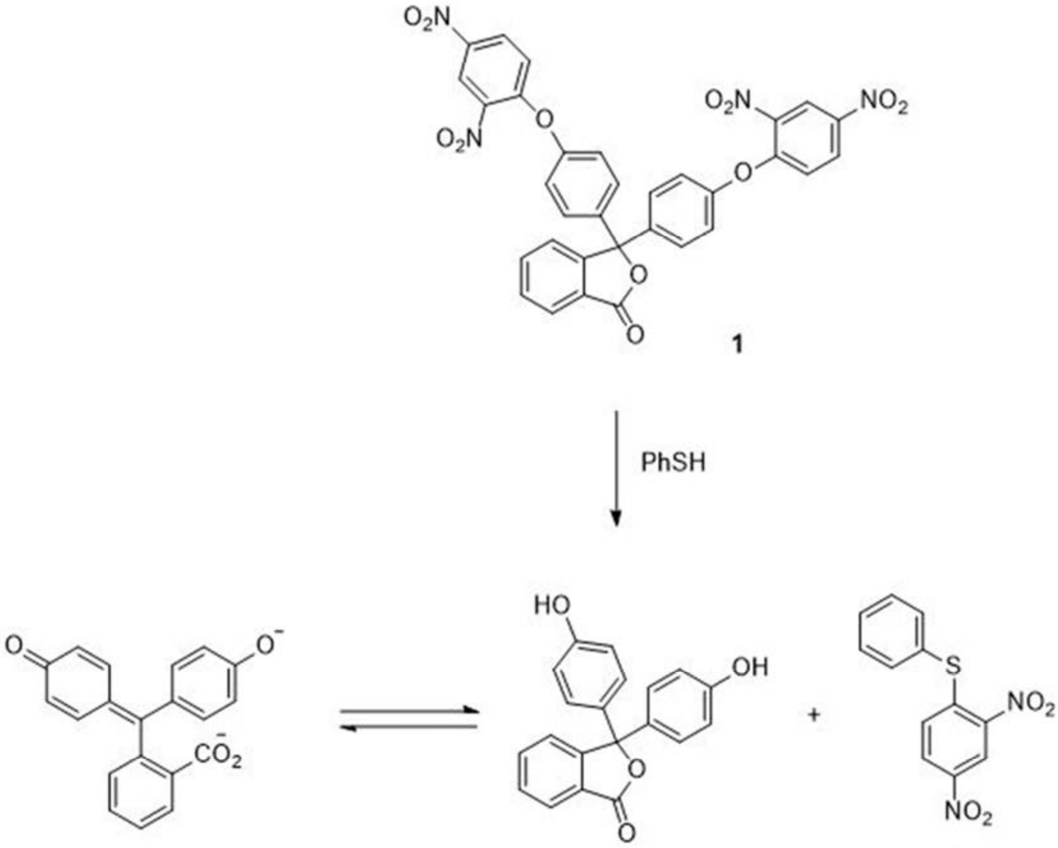
A Colorimetric Detection of Thiophenol based on a Phenolphthalein Derivative and Its Application as a Molecular Logic Gate

권나현 윤주영[1,*] 이다영

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

A phenolphthalein-based colorimetric probe bearing dinitrobenzene group is reported as a thiophenol (PhSH)-selective chemodosimeter. PhSH can react with chemodosimeter 1 to afford phenolphthalein. The addition of PhSH to the aqueous solution of 1 followed by a changing pH of the resulting solution to basic induced a selective color change from colorless to pink. Furthermore, using PhSH and base as inputs and color change of 1 by naked eye as an output, an AND logic gate was constructed.



1

Pink
pH 8.2-12.0

2
colorless

3

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Novel One-component Organocatalysts for the Coupling of Carbon Dioxide and Epoxides

김요셉 김민 김정곤[1] 김영조[*]

충북대학교 화학과 [1]전북대학교 화학과

이산화 탄소와 에폭사이드로부터 합성되는 cyclic carbonate 는 많은 응용성을 가지는 유용한 화합물로 알려져 있다. 이러한 cyclic carbonate 합성에는 보통 금속을 포함하는 산촉매와 아이오딘화 이온과 같은 친핵체가 쌍을 이룬 형태의 촉매가 많이 이용된다. 이산화 탄소의 C1 source 로서의 화학적 전환에 있어서의 환경 및 에너지 측면에서 여전히 유기 촉매는 비효율적이라고 알려져 있다. 즉, 유기 촉매를 사용하여 cyclic carbonate 을 효율적으로 합성하기 위해서는 높은 온도, 긴 반응 시간 및 많은 양의 촉매가 필요하다고 알려져 있다. 따라서 이러한 문제점을 극복하기 위하여 본 연구에서는 수소 결합의 시너지 효과를 통해 유기 촉매이면서 상온과 적은 양의 촉매만을 사용하여 이산화 탄소와 에폭사이드의 커플링 반응을 수행한 결과를 발표하고자 한다.Acknowledgment: 본 연구는 지역혁신창의인력양성사업(2014H1C1A1066874)의 지원을 받아 수행되었음

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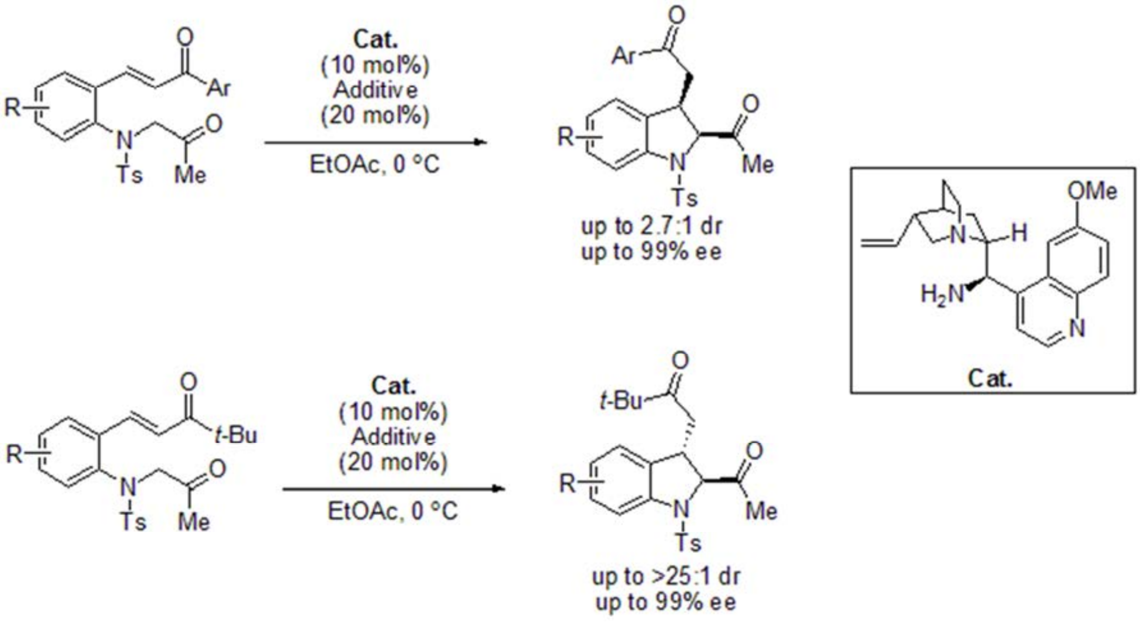
Enantioselective synthesis of 2,3-disubstituted indolines via an asymmetric organocatalytic intramolecular Michael addition

이주성 고광민 김성곤*

경기대학교 화학과

The enantioselective synthesis of 2,3-disubstituted indolines has been developed through an organocatalytic intramolecular Michael addition. Employing primary amine derived from chinchona alkaloid as the catalyst, the intramolecular cylization reaction of (E)-3-(2-(2-oxopropylamino)aryl)-1-arylprop-2-en-1-ones proceeded to generate the corresponing cis-2,3-disubstituted indoline derivatives in high yield, with moderate diastereoselectivities and excellent enantioselectivities (up to 2.7:1 dr, up to 99% ee). Moreover, the catalytic reaction of (E)-3-(2-(2-oxopropylamino)aryl)-1-akylprop-2-en-1-ones afforded trans-2,3-disubstituted indolines in high yields with good to excellent diastereo- and enantioselectivities (up to 20:1 dr, up to 99% ee).



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Efficient Continuous Flow Synthesis of 1-Sulfonyl-1,2,3-Triazole Preparation

권용주 김원석[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학 나노과학과

1-Sulfonyl-1,2,3-triazoles, the electron-deficient heterocycles, are used as convenient reactive azavinyl carbenes. With their weakened N1-N2 bond, they promote the ring-chain isomerism in formation of diazoimine. Various batch-type methods for synthesizing 1-sulfonyl-1,2,3-triazoles have been reported. However, most reaction conditions for these methods require long reaction time. Herein, an efficient method for the synthesis of 1-sulfonyl-1,2,3-triazoles is described with short reaction time. The reaction was carried out in excellent yield by using an flow synthesis system.

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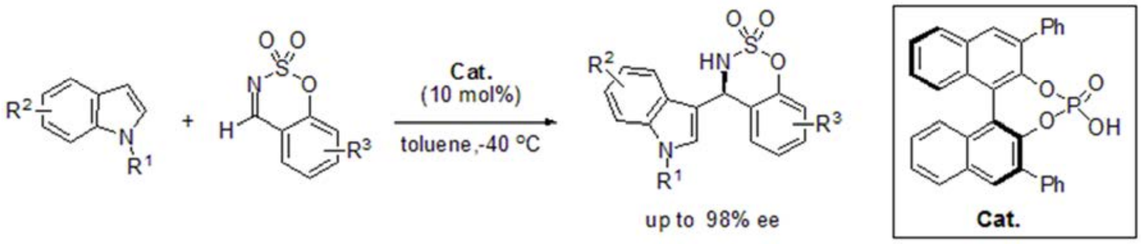
Organocatalytic enantioselective Friedel-Crafts reaction of indole with cyclic N-sulfimines

이상규 김성곤*

경기대학교 화학과

An asymmetric organocatalytic Friedel-Crafts reaction of indole with benzoxathiazine 2,2-dioxides has been developed. Chiral phosphoric acids are enanantioselective catalysts for Friedel-Crafts reaction affording the corresponding 3-indolyl sulfamidates in good yields and with high enantioselectivities (up to 98% ee) for a broad range of functional groups and substitution patterns.



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The use of *N*-formyl/acyl sulfenamide for the sulfenylation of carbonyl compounds

노형완 장혜영[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 화학과

Chemicals involving sulfur-nitrogen bond are widely used as a building block in pharmaceutical and industrial processes. They are also used as a sulfur group transfer reagent in organic synthesis. Recently, we reported the catalytic synthesis of sulfenamides using thiols by using sulfenamides, various carbonyl compounds were converted to α-sulfenylated compounds in good yields. In this study, the detailed sulfenylation conditions along with the reactivity comparison of various sulfonamides are presented.

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Yb-catalyzed synthesis of sulfinates using thiosulfonates

손수빈 장혜영[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 화학과

Sulfinates are commonly used for the synthesis of various organosulfur compounds which are employed in organic synthesis, medicinal chemistry and monomer of polymerization. Known synthetic methods of sulfinates are 1) coupling of sodium sulfinates with alcohols, and 2) coupling of sulfonyl chlorides with alcohols. These methods have limitations of using stoichiometric amounts of Lewis acids and of using relatively unstablility of sulfonyl chlorides. Compared to these methods, in this study, we present the coupling of relatively stable and easily prepared thiosulfonates with alcohols in the presence of ytterbium catalysts, to afford the desired sulfinates in modest to good yields.

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Simple modification of basic dyes with bulky & symmetric WCAs for improving solubilities in organic solvents without color change

우성윤 김재필[1,*] 이재문 노정우[2]

서울대학교 재료공학과 [1]서울대학교 재료공학부 [2]서울대학교 공과대학 재료공학부

Basic dyes are popularly used commercial dyes due to their obvious advantage in optical property and price competitiveness. Basic dyes usually show superior solubilities in water, but, they are rarely dissolved in organic solvents due to their ionic characteristics. This makes it hard to use the basic dyes as colorants of electronic devices. To overcome this solubility problem of basic dyes, a simple and easy solubility enhancement of basic dyes was performed with bulky and symmetric weakly coordinating anions (WCAs). The WCAs decreased the ionic character of the dyes by broadening the partial charge distribution and causing a screening effect on the ionic bonding. This new modification with WCAs has advantages in that it has no influence on the optical properties of the dyes. The solubilities of unmodified and modified dyes were tested in several organic solvents. X-ray powder diffraction patterns of the dyes were measured. Color films were prepared with the dyes and their color loci were analyzed to evaluate the optical properties. By the modification with WCAs, commercial basic dyes showed sufficient solubilities for being applied to various applications while preserving their superior optical properties.

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A New Approach to Examine the Formation of Amyloid Oligomers Using Quartz Crystal Microbalance

송하은 신재호 최의진[1] 강경태[*] 이진석[1,*]

경희대학교 응용화학과 [1]숙명여자대학교 화학과

Amyloid oligomer is an intermediate species within amyloidogenesis and funtions as a precursor of amyloid fibrils. In Alzheimer's disease, many evidences have supported that soluble $A\beta_{1-42}$ oligomers, rather than $A\beta_{1-42}$ fibrils, are a main cause of neurotoxicity. However, it has been difficult to identify and analyze these soluble $A\beta_{1-42}$ oligomers, and the pathology of Alzheimer's disease remained incompletely explained except a few uncertain hypotheses and partial evidences. In this respect, a new way of looking into dynamic kinetics and chemical structures of soluble oligomer is suggested based on the use of Quartz crystal microbalance(QCM). $HS\text{-}(CH_2)_m\text{-}EG_n\text{-}OCH_2\text{-}COOH$ was used to deposit proteins on a self-assembled monolayer and prevent abnormal deposition simultaneously. We used amyloid monomer-immobilized mixed SAMs of $HS\text{-}(CH_2)_{11}\text{-}EG_3\text{-}OCH_2\text{-}COOH$ and $HS\text{-}(CH_2)_{11}\text{-}EG_2\text{-}OCH_2\text{-}OH$) as a probe for QCM analysis, and used this chip to monitor the mass growth of amyloid species, which reflected the transition from monomers to oligomers, and in turn to fibrils. In this way, we could explore the dynamic kinetics of overall amyloid fibrosis and compare the results with previous oligomer studies to determine the appearance and duration of specific oligomers.

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Synthesis of Aromatic PAMAM Dendrimer containing Carbazole as a core Chromophore

우수근 이재욱*

동아대학교 화학과

Click chemistry, which is the Cu(I)-catalyzed Huisgen dipolar cycloaddition reaction between an organic azide and a terminal alkyne, has found many applications in combinatorial and organic chemistries, material science, and synthesis of polymer and dendrimer. The click chemistry as a concept of simplifying synthesis is very useful tool to produce functional polymers and dendrimers. The reaction, characterized by very high yields, mild and simple reaction conditions, excellent oxygen and water tolerance, and simple product isolations, is highly chemoselective affording only the desired 1,2,3-triazole even in the presence of a large variety of other functional groupsWe are pay attention to this fact to investigate the synthetic method of dendrimer using the Huisgen dipolar cycloaddition reaction. The synthetic strategy for convergent synthesis of emissive Aromatic PAMAM Dendrimers having the core chromophore via the copper-catalyzed 1,3-dipolar cycloaddition reaction between alkyne and azide was described. 3,6-diethynyl-9H-carbazole, designed and synthesized to serve as the core in dendrimer, was stitched with the azide-functionalized Aromatic PAMAM dendrons by the click chemistry leading to the formation of fluorescent PAMAM dendrimers in high yields. The absorption and emission of the dendrimers were investigated. All dendrimers are characterized by NMR, IR, UV-Vis, PL and GPC analysis.

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A general, rapid, and efficient method for basic dyes removal from wastewater with bis(trifluoromethylsulfonyl)imide anion

우성윤 김재필[1,*] 이재문 노정우[2]

서울대학교 재료공학과 [1]서울대학교 재료공학부 [2]서울대학교 공과대학 재료공학부

Methods of removing dyes dissolved in wastewater has been extensively studied. However, most of the proposed solutions are uneconomical, take a long time, or show low efficiency. Basic dye is a type of widely used commercial dye of which solubility in water is drastically changed by introduced counteranion. Degree of solubility change highly depends on the type of introduced counteranion. Thus, basic dyes dissolved in wastewater could be easily precipitated by introduction of proper counteranion.Eight basic dyes were paired with bis(trifluoromethylsulfonyl)imide anion. The chosen anion is generally known for an efficient compound to replace the initial counteranion of basic dyes. After precipitated basic dyes in water were filtrated, removal efficiencies were assessed by comparing extinction coefficient of the filtrate with that of unsubstituted basic dye solution. In addition, transmittances of filtrate and unsubstituted basic dye solution were compared. Each of eight basic dyes showed high removal efficiency of over 99 percent within thirty minutes.

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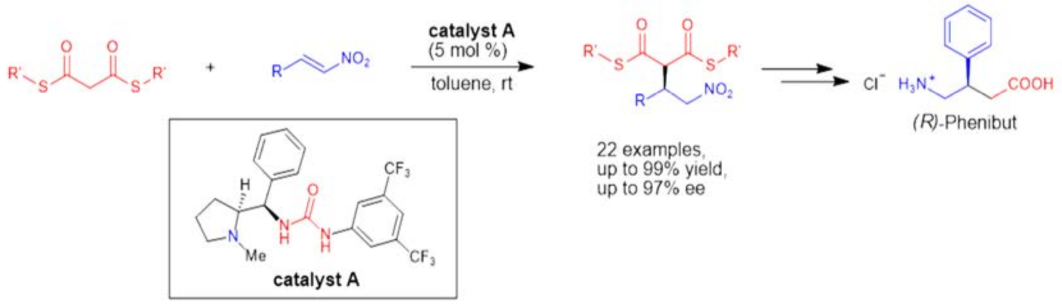
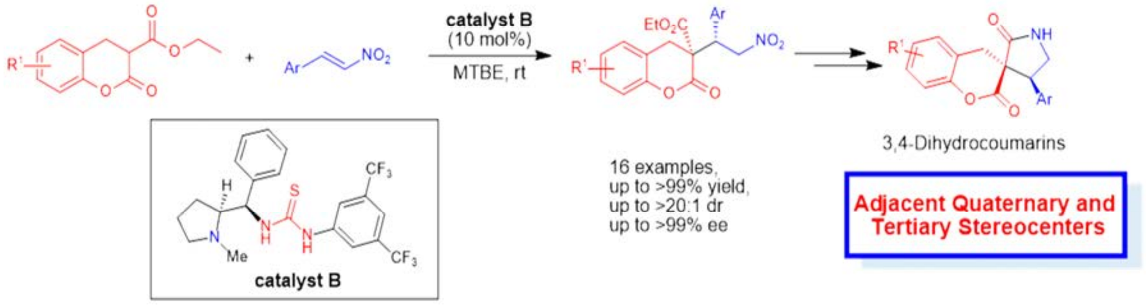
Asymmetric Michael Addition Reactions of trans-β-Nitroolefins Catalyzed by Novel L-Proline Derived Bifunctional Organocatalysts

JINHUI 김승태 조수민 이주열 최유나 류도현*

성균관대학교 화학과

The organocatalytic asymmetric Michael addition of various nucleophiles with nitroolefins represents a convenient route to highly functionalized synthetic building blocks in organic synthesis. Recently, our group developed a series of novel L-proline derived tertiary amine bifunctional organocatalysts, which were successfully applied to the asymmetric Michael addition of dithiomalonates to trans-β-nitroolefins.1 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)-phenibut in high yield. As a continuation of this work, an asymmetric Michael addition of 2-oxochroman-3-carboxylate esters to trans-β-nitroolefins was developed. 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. The adduct was further transformed to a spiro-dihydrocoumarin compound in three steps with good yield.2 References1. Jin, H.; Kim, S. T.; Hwang, G. S.; Ryu, D. H. J. Org. Chem. 2016, 81, 3263-3274.2. Jin, H.; Cho, S. M.; Hwang, G. S.; Ryu, D. H. Adv. Synth. Catal. 2017, 359, 163-167.


catalyst A
(5 mol %)
toluene, rt
R'
S
O
R
NO₂
H
N
Me
CF₃
catalyst A
22 examples,
up to 99% yield,
up to 97% ee
Cl⁻
H₃N⁺
COOH
(R)-Phenibut


catalyst B
(10 mol%)
MTBE, rt
R'
O
Ar
NO₂
EtO₂C
NH
S
H
N
Me
CF₃
catalyst B
16 examples,
up to >99% yield,
up to >20:1 dr
up to >99% ee
3,4-Dihydrocoumarins
Adjacent Quaternary and
Tertiary Stereocenters

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Pd-catalyzed polymerization using CO and ethylene; the effect of heterogeneous acid additives

정연주 임유나 강신영[1] 손성욱[1,*] 장혜영[2,*]

아주대학교 에너지시스템학부 [1]성균관대학교 화학과 [2]아주대학교 화학과

The use CO gas as a C1(Carbon monoxide, Carbon dioxide, and methane) chemical feedstock would be a possible solution to reduce the level of global warming gas. For example, thermoplastic polyketones which attract great attention to the polymer industry due to its high impact strength and chemical resistance have been synthesized from CO and ethylene in the presence of a palladium catalyst. Current synthetic methods of polyketones involve problems like reactor fouling issue. In this presentation, we present a new polyketone catalyst composition involving Pd catalysts and PS(Polystyrene)-SO_3H, where the reactor fouling was resolved by PS-SO_3H. Detailed reaction conditions and the effect of PS-SO_3H are discussed.

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Design of a Glucose Uptake Sensor and Its Application to Primary Hippocampal Neurons

김윤영 성준[1] 강경태[*] 김은하[1]

경희대학교 응용화학과 [1]아주대학교 분자과학기술학과

Glucose plays an important role as a primary fuel in a variety of vertebrate and invertebrate cells. Understanding how, when, and where glucose is absorbed by a cell is, therefore, critically important in elucidating its biological functions and their ramifications. In this work, we designed a molecule with which we could sense glucose uptake by primary hippocampal neurons. Fluorescent dye (silicon rhodamine) conjugated with glucose, having a near-infrared fluorescence window, was found to be absorbed by hippocampal neurons in a competing fashion with normal glucose. We quantified the amount of glucose uptake by comparing fluorescence intensities and studied the exact mechanism of the uptake. The suggested glucose uptake sensor will provide valuable information on biological roles of glucose in neuronal growth.

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장소: 일산 KINTEX
발표코드: **ORGN.P-358**
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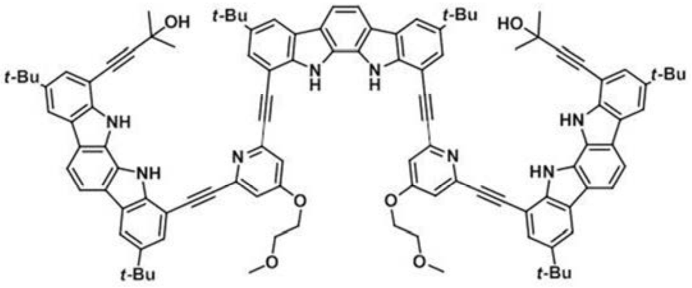
A Fluorescent Anion Sensor based on Indolocarbazole-Pyridine Hybrid Foldamer

장한빛 정규성*

연세대학교 화학과

In recent years, many efforts have been devoted to the development of anion sensors because anions play many important roles in chemical, biological and environmental systems. Herein, we have been prepared foldamer 1 that consists of indolocarbazoles and pyridines linked alternatively through ethynyl bonds. Foldamer 1 is fluorescent in an unfolded conformation, but its fluorescence is completely quenched in a folded conformation. Foldamer 1 shows a turn-off fluorescence response because it folded to a helical conformation in water-saturated CH2Cl2, whereas it shows a turn-on fluorescence response drastically in the presence of anions because it disturbs the folded conformation to avoid repulsion with non-bonding electrons of pyridyl nitrogen. Also, the ethylene glycol groups (Eg) of pyridine make it easier by increasing the non-bonding electron density of pyridyl nitrogen. The binding properties of foldamer 1 were investigated by 1H NMR and Fluorescence spectroscopy. This result has been further extended to develop a fluorescence sensor for anions. Details will be described in the presentation.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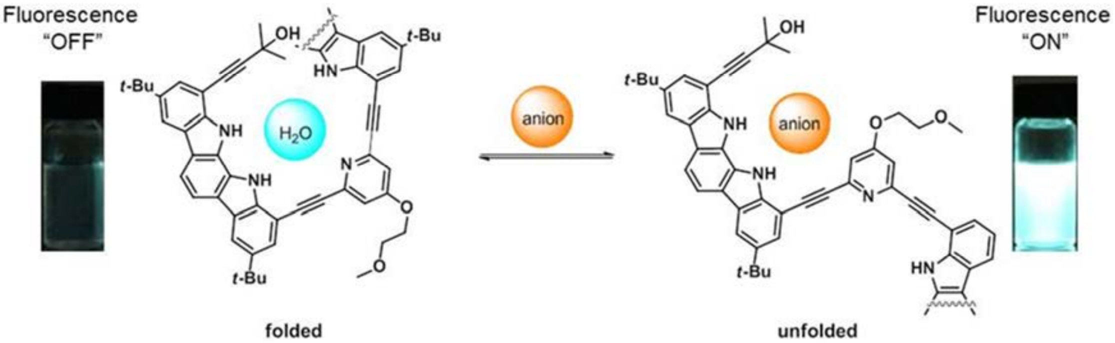
foldamer 1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t-Bu
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Fluorescence
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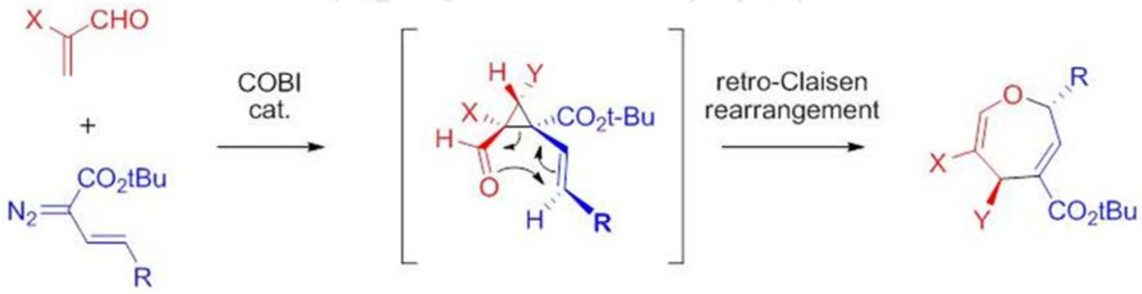
Catalytic stereoselective synthesis of 2,5-dihydrooxepine via retro-Claisen rearrangement

조수민 JINHUI 남동국 김재연 이주열 류도현*

성균관대학교 화학과

Recently, seven-membered oxacycles become more important compounds due to their occurrence in natural products, usage in polymers and pharmacological applications. For these reason, many synthetic methods for the formation of seven-membered oxacycles have been developed. However, there is few synthetic method of 2,5-dihydrooxepine as not only racemic but also chiral. In this research, we developed catalytic enantioselective synthetic method of 2,5-dihydrooxepine via retro-Claisen rearrangement which contains vinylcyclopropanecarboxyaldehyde as intermediate.



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발표코드: **ORGN.P-360**

발표분야: 유기화학

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Synthesis and characterization of novel propeller shaped diketopyrrolopyrrole(DPP) organic dyes with different length of alkyl chain moieties for enhanced aggregation induced emission(AIE)

이재문 노정우[1] 김재필[2,*] 황태규[2] 우성윤

서울대학교 재료공학과 [1]서울대학교 공과대학 재료공학부 [2]서울대학교 재료공학부

Fluorescent molecules in the solid states have been extensively studied for applications in gas sensor and organic light emitting diode (OLED). However, most of fluorescent molecules that exhibit large fluorescence in solutions have low fluorescence or even non-emission in the solid states. Such an emission quenching is usually attributed by their intermolecular interaction, In order to improve fluorescence in solid state, propeller-shaped fluorogens with aggregation-induced emission (AIEgen) characteristics have been designed. And alkyl chain has been introduced into the fluorogens to find out the relation between length of alkyl chain and optical properties in solid state.

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Black to transparent electrochromic window with metal oxide nano particles in ionic gel

이우재 김영훈 김진보 박치현 김은경*

연세대학교 화공생명공학과

Electrochromic window has gained much interest due to their wide variety of applications, including smart windows, chemical sensors, transparent displays and light modulators. Using light scattering effect of metal oxide nano particles, an electrochromic window with a scattering layer was prepared on a transparent electrode. Upon reduction of meta ions the electrochromic scattering layer turned into black, which was switched into transparent upon oxidation. The reversibility and color contrast of the black electrochromism were optimized by controlling applied potential and composition of ionic gel.

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A study on improving thermal stability and dispersibility of LCD color filter by introducing ionic interaction between heat resistant cationic phthalocyanine dyes and an anionic binder

이재문 김재필[1,*] 이우성[2] 황태규[1] 우성윤

서울대학교 재료공학과 [1]서울대학교 재료공학부 [2]한국생산기술연구원 ICT섬유의류그룹

LCD color filter containing soluble organic dyes have a dye aggregation issue during baking process which induces low transmittance of the color filter. Therefore, strategy to keep dispersed state of the dyes is required.In this study, we enhanced affinity between dyes and binder that are major components of millbase by their electrostatic attraction. Cationic phthalocyanine dyes were synthesized and anionic binders were polymerized for this purpose. Solubility and thermal stability of the dyes were improved by alternating their counter ions from iodine to bulky anionic compound. Ionic films composed of ionic dyes and binder showed high thermal stability and contrast ratio compared to non-ionic films fabricated with non-ionic dyes and binder. Structure analysis of the synthesized dyes and binders were confirmed by elemental analysis, mass, gel permeation chromatography and IR-spectroscopy. Optical and thermal properties of the dyes were investigated by UV-visible spectrometer and TGA in comparison with iodo-phthalocyanines.Consequently, highly dispersed dye based color filters were developed with ionic dyes and binder. Particle size of the ionic films were maintained after baking process and contrast ratio of the films were higher than that of non-ionic films.

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Effect of Planar D-D-π-A Metal Free dyes on Thin-Film dye sensitized solar cells

남동국 김승태 조수민 최유나 이주열 류도현* 권태혁[1]

성균관대학교 화학과 [1]UNIST 친환경에너지 공학부

The dye-sensitized solar cells have been The planarity of metal free organic dyes is one of important factors for intramolecular charge transfer (ICT) and power conversion efficiency of dyes. We designed and synthesized D-D-π-A Metal Free dyes introducing carbazole, indoline, quinoline units to control planarity. The power conversion efficiency (PCE) of planar dyes got higher efficiency and faster ICT values. Therefore, RK-3 dyes indoline units, double donor and planar pstructure exhibits PCE of 10.3% when active film thickness is 3.5 μm.

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Asymmetric Formation of β-Hydroxysilane Using Diazo Compounds and Aldehydes

김재연 JINHUI 김승태 조수민 이주열 류도현*

성균관대학교 화학과

α-Silyl ketones are useful building blocks for organic synthesis because they are good substrates for many regio- and stereoselective reactions to construct carbon-carbon and carbon-heteroatom bonds in high stereoselectivities[1]. 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[2]. In this research, we developed highly enantioselective method for the synthesis of β-hydroxysilane reduced from α-silyl ketone catalyzed by chiral boron catalyst. The synthetic utility of this method was demonstrated by the synthesis of allylic silanes which are very versatile synthetic reagents for the regioselective introduction of the allyl group into electrophiles[3].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, 1498.3. Hosomi, A. Acc. Chem. Res. 1988, 21, 200

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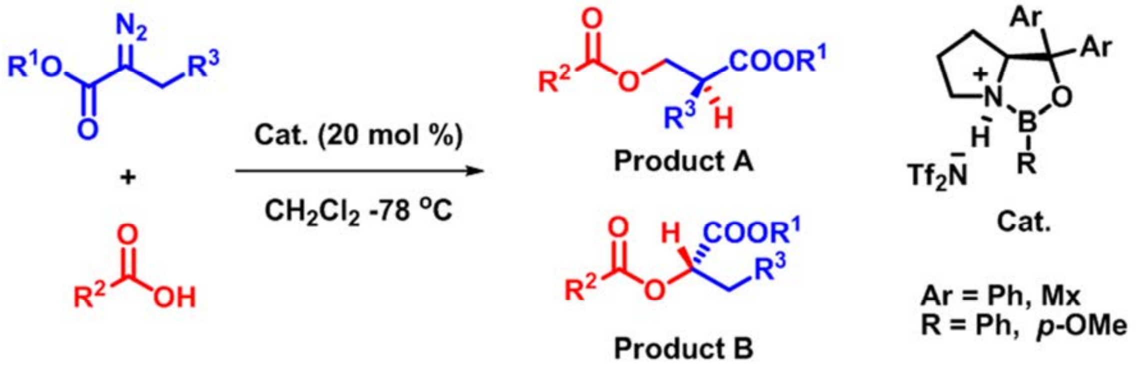
Enantioselective O-H Insertion of α-Benzyl Diazoesters by Chiral Oxazaborolidinium Ion-Activated Carboxylic Acids

김승태 JINHUI 김재연 남동국 최유나 류도현*

성균관대학교 화학과

The asymmetric O-H insertion reaction is an fascinating method for preparing tertiary chiral carbon centers, usually found in valuable building blocks of biologically active natural products. In this research, A new type of chiral proton donor which is combined with chiral Lewis acids assisted Brønsted Acids (chiral LBAs) and carboxylic acid will be discussed. This new chiral proton donor is highly effective reagent for asymmetric O-H insertion reaction. The reaction proceeded in good yields (up to 97%) with excellent enantioselectivities (up to 99% ee).



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New Aromatic Heterocyclic Oligomers: Synthesis, Characterization and Properties

김성수 김인태*

광운대학교 화학과

We have studied various conjugated oligomers that is synthesized to make conjugated polymers. Conjugated polymers have used as a substantial compound for a variety of application. Conjugated oligomers also have similar properties to conjugated polymers from the merits of demerits. In this work, we compared several oligomers synthesized in our laboratory. The structure of the compounds was identified by ^{1}H NMR, ^{13}C NMR, and FT-IR spectroscopy. We also posted each UV/Vis absorption, photoluminescence(PL) spectra for the synthesized the compounds. Through this work, we can check the efficiency of each oligomers and it is expected to be applied to the photovoltaic devices, light emitting diodes (LEDs), field effect transistors (FETs), and electrochromic devices, etc.

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Magnetite and titanium carbide coated unwoven carbon fiber fabric for enhanced performance in EMI shielding and thermal conductivity

한지훈 RAMANASKANDA BRAVEENTH 주미라 채규윤*

원광대학교 화학과

Electromagnetic interference (EMI) is a radiated electromagnetic signal-intrusion generated by an external source which can affect and perturb the functioning of nearby electronic equipment such as circuits. The rapid development of modern electronic products which results in abundant use of electronic devices and highly integrated circuits generate significant amounts of electromagnetic radiation, thus producing adverse effects on highly sensitive, precision electronic equipment and also living beings. EMI shielding is crucial to protect humans and circuits from EMI radiation. Traditionally many metal composites materials such as iron, copper and aluminum have been used either as conductive fillers for composites or base material for films because of their high electrical conductivity, superior electrical density, and large aspect ratio. In current study a carbon fiber based fabric coated with magnetite(Fe_3O_4) and titanium carbide(TiC) was developed. This shows high EMI shielding effectiveness over 30 dB with the maximum of 33.6 dB and 36.8 dB for copper coated and iron coated one respectively with the thickness of the fabric about 150-200 μm. Furthermore, this coating gave rise to increased tensile strength and thermal diffusivity.

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Pd-NHC Catalyzed Bisalkoxycarbonylation of Olefins

임유나 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Diesters are precursors that can be converted into intermediates, solvents, and polymeric monomers for the synthesis of pharmaceuticals. They can be used not only in the pharmaceutical industry but also in the overall chemical industry. This study proposes a method for the synthesis of succinic acid diesters, which are a high value added material, through the carbonylation of relatively low value added materials such as ethylene and carbon monoxide. The succinic acid diesters are synthesized through the alkylation of succinic acid, and succinic acid can be synthesized industrially from the hydrogenation of maleic acid, oxidation of 1,4-butanediol, and the carbonylation of ethylene glycol. These syntheses are not economically efficient due to the multiple steps of reaction. Therefore, the direct synthesis of succinic acid diesters by the carbonylation of ethylene using palladium catalysts both reduces the complex experimental steps and also is an atomic economic reaction. In this study, succinic acid diesters are synthesized by introducing a novel N-heterocycle (NHC) carbene into palladium catalysts.

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Transition metal-free C-S coupling : synthesis of vinyl sulfones

황상준 장혜영[1,*]

아주대학교 에너지시스템학부 [1]아주대학교 화학과

Organosulfur compounds are used in pharmaceuticals, agrochemicals, materials, and as intermediates in organic synthesis, and they often appear abundantly in biological systems. The formation of C-S bonds, in particular vinyl sulfones is important in pharmaceutical industries. For examples, K11777 is used a potent inhibitor of parasitic and mammalian proteases. There are many ways to synthesize vinyl sulfones, but most of previous methods suffer harsh reaction conditions, intractable starting materials, and complicated procedures. Thus, it is necessary to developthe more efficient synthesis of vinyl sulfones. In this study, the transition metal free synthesis of vinyl sulfones using stable and easy to handle thiosulfones was proposed.

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Improving contrast ratio of LCD by enhancing dispersion performance: new phthalocyanine derivatives as synergist

노정우 김재필[1,*] 이재문[2] 황태규[1] 우성윤[2]

서울대학교 공과대학 재료공학부 [1]서울대학교 재료공학부 [2]서울대학교 재료공학과

The color filter is one of the most important parts to show images and it determines color properties of LCD. The color properties of color filter depend on pigment properties. The contrast ratio also depends on light scattering of pigment particles and large particle size of pigment increase light scattering. The synergist interacts with dispersants and pigments, it thus supresses aggregation and improves dispersion of the pigment particles. Here, phthalocyanine dyes have amine, ester, and carboxyl group as green synergists were synthesized. Their thermal, spectral properties and particle size were examined by TGA, UV-Vis spectroscopy, particle size distribution analyser, and scanning electron microscopy respectively. Consequently, the contrast ratio increased by adding the synthesized synergists and the phthalocyanine derivatives as synergists could effectively improve the performance of liquid crystal display.

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Synthesis, characterization, and application for reducing thickness of the color filter

노정우 김재필[1,*] 이재문[2] 황태규[1] 우성윤[2]

서울대학교 공과대학 재료공학부 [1]서울대학교 재료공학부 [2]서울대학교 재료공학과

Four green phthalocyanine dyes were synthesized to improve the optical performance and decrease thickness of liquid crystal display color filters. Among them, dyes of isomeric substituted phthalocyanines were more soluble in PGMEA and tetra aryloxy-dodeca chloro-substituted zinc phthalocyanine showed superior spectral and chromatic properties. Their thermal properties were examined by thermogravimetric analysis. Dye-based color filters were also fabricated using the synthesized dye. The spectral properties and thermal stability of the color filters are investigated by comparing them with pigment-based color filter. The prepared color filters showed superior spectral properties due to high absorbance of dyes. Their thermal stability was also similar to those of the pigment-based color filters. The results showed that the prepared dye could be successfully reduce thickness of liquid crystal display color filter.

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Application of double addition chemistry on dihydroisoquinolines: Concise synthesis of methopholine and homoprotoberberine

김슬기* 최유리[1] 황종연 손정훈[2] 김필호

한국화학연구원 의약화학연구센터 [1]과학기술연합대학원대학교(UST) 의약화학 및 약리생물학 [2]충남대학교 화학과

Alkaloids containing dihydroisoquinoline (DHIQ) or tetrahydroisoquinoline (THIQ) have been traditionally a rich resource of pharmaceutics. Biological properties of DHIQ or THIQ alkaloids are ranging from antihypertensive, anti-inflammatory, antiulcer, and anti-leukemic activities. Double addition chemistry of alkyl halides on 1-methyl-3,4-DHIQ was discovered. This reaction was compatible with various alkyl halides and DHIQs. Application of this chemistry on the total synthesis of natural products was pursued to develop a novel synthetic pathway for the preparation of methopholine using double addition of alkyl halides on 1-methyl-3,4-DHIQ, far more effective methodologies compared with known methods. In a similar context, a novel synthetic route for tetracyclic alkaloids containing THIQ, such as homoprotoberberine, was discovered using tandem alkylation and intramolecular cyclization on 1-methyl-3,4-DHIQ. Diverse homoprotoberberine analogs have been prepared utilizing various 1,2-bis(bromomethyl)benzenes.

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Synthesis of BISESAMOL Derivetives via Diastereomeric Resolution Using a Boronic Acid Moiety as a Resolving Group

조영인 정연지 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 chiral building blocks in chiral Brønsted acid catalysis. 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 the diastereomeric resolution of BISESAMOL boronic acid using a boronic acid moiety as a resolving group. Subsequent derivatization of the boronic acid moieties 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, 81, 8464.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **ORGN.P-374**
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Development of a Novel Synthetic Route for Indoloquinolizine Scaffold via Intramolecular Imino-Stetter Reaction

박은준 천철홍*

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. One of the most common methods to access the core indoloquinolizine structure is the Pictet-Spengler reaction of imines derived from tryptamine and aldehydes. Another one is the Bischler-Napieralski reaction of 3-piperidioneindole derived from tryptamine and furancarboxylic acid. However, these methods generally require additional steps to generate another six-membered ring and toxic metals for coupling reactions.Recently, our group developed a new method for the synthesis of 2-substituted indole-3-acetic acid derivatives from aldimines derived from 2-aminocinnamic acid derivatives and aldehydes via cyanide-catalyzed intramolecular imino-Stetter reaction. 1,2 We further extended this protocol to the synthesis of indole-3-acetic acid derivatives bearing a pyridyl moiety at the 2-position from aldimines obtained from 2-aminocinnnamic acid derivatives and various pyridinecarbaldehydes. Subsequent reduction of the carboxylic acid moiety to an alcohol followed by cyclization to provide tetrahydro-indoloquinolizines. Following reduction of the pyridinium ring with several nucleophiles afforded the expected indoloquinolizines. In this poster, we will describe our new approach towards the preparation of indoloquinolizine scaffold. Reference1. Lee, S. J.; Seo, H.-A.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 1566.2. Seo, H.-A.; Cheon, C.-H. J. Org. Chem. 2016, 81, 7917.

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발표코드: **ORGN.P-375**
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Concise Total Synthesis of Paullone and Kenpaullone via Cyanide-Catalyzed Intramolecular Imino-Stetter Reaction

이상은 천철홍*

고려대학교 화학과

Paullone, originally known as a class of potent cyclin dependent kinase (CDK) inhibitors, has shown to display various biological activities with further research. Particularly, since a substituent at the C-9 position of paullone turned out to have a significant impact on the biological activities, several derivatives carrying a different substituent at the C-9 position have been developed to date. In order to fully investigate the structure-activity relationships of paullone derivatives, several synthetic approaches toward paullone and its derivatives has been developed. Among the methods developed, one of the most popular methods is Fischer indole synthesis. Alternatively, the target molecules could be prepared from indole-3-acetic acid derivatives via the C-2 arylation followed by lactam formation. However, most of the former synthetic approaches require relatively lengthy steps. Very recently, we developed a method to access 2-aryl indole-3-acetic acid derivatives from aldimines, derived from 2-aminocinnamic acids and aromatic aldehydes, through the cyanide-catalyzed imino-Stetter reaction. 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 a benzaldehyde derivative bearing either amino group or its precursor at the ortho-position. In this presentation, we will describe the synthesis of paullone and kenpaullone via imino-Stetter reaction of aldimine from methyl 2-aminocinnamate derivatives and 2-nitrobenzaldehyde followed by treatment of the resulting indole-3-acetate with Zn under acidic conditions. Upon the reduction of the nitro group into amino group under these conditions, the resulting amino group spontaneously underwent lactam formation leading to paullone and kenpaullone in only two steps from commercially available starting materials.

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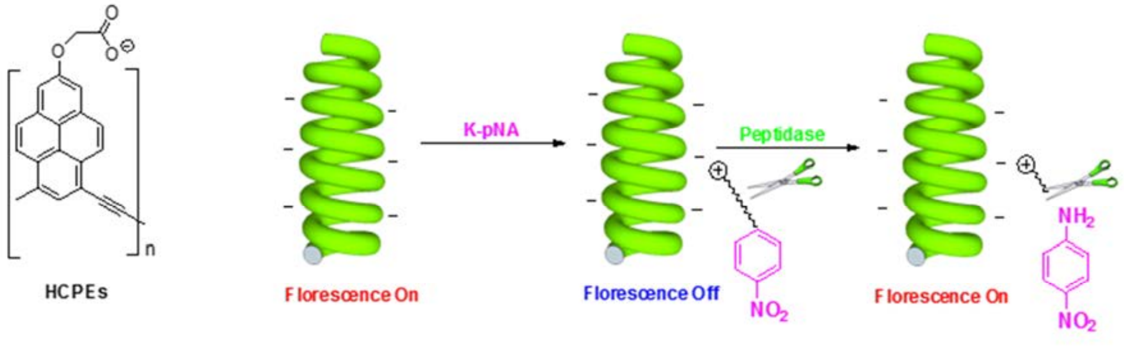
Highly Sensitive Chemosensor Based on Helical Conjugated Polyelectrolytes

이선우 이정무 이성호*

대구대학교 화학응용화학과

A highly efficient chemosensor based on the helical conjugated polyelectrolytes (HCPEs) has been designed and synthesized. HCPEs display intramolecular self-assembly with helical formation in aqueous solution, giving rise to strong excimer emission. We found that more efficient excimer quenching in aqueous solution is caused by energy migration through the pyrene aggregates as well as conjugated backbones. This is because the delocalized excited state of the pyrene stack is mobile as in the case of covalently linked conjugated backbone. That is, the molecular aggregation controls exciton transport and amplified quenching phenomena. For the bioanalytical applications, the activity of peptidase was successfully monitored by real-time turn-off assay.



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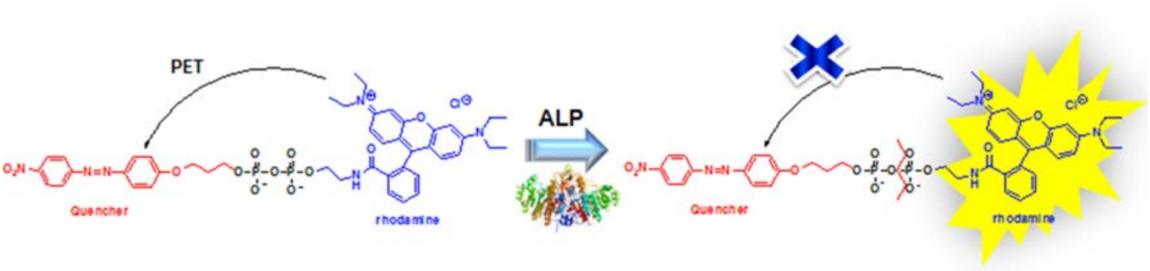
A Promising Fluorescent Probe for Real-Time Monitoring of Alkaline phosphatase (ALP) Activity

정수진 이성호*

대구대학교 화학응용화학과

We report the fluorogenic detection of the alkaline phosphatase (ALP) in aqueous buffer solution. This is achieved by “Sense-Break-Display” system, employing phosphate groups-decomposing probes that contain pyrophosphate moiety designed to induce bimolecular decomposition by the enzymatic action. The activity of alkaline phosphatase (ALP) was successfully monitored by real-time turn-on assay.



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Aromaticity in Bicyclic Doubly N-fused Bithiophene-bridged Octaphyrin

조선희 양윤재 박정수*

숙명여자대학교 화학과

During several decades, there has been great interest and substantial efforts in the synthesis and characterization of expanded porphyrin derivatives for a variety of practical applications, including optoelectronic devices, nonlinear optical (NLO), and photodynamic therapy (PDT) materials. In order to control their electronic and spectral properties, various synthetic modifications have been also applied, including changes in the number and nature of core sub-aromatic and meso-bridging moieties, ring-fusion/confusion, and introduction of internal bridging moieties[1]. Among these, internally bridged core-modified expanded porphyrins has been recently recognized as a new method to create dual aromaticity and efficient way to modulate the molecular conformation and p-conjugation of expanded porphyrins[2]. In this study, we synthesized, for the first time, a new type of bicyclic doubly N-fused expanded porphyrin derivative as shown in **Figure 1**. The molecular structure was fully characterized by X-ray crystallography as well as NMR, and Mass analyses. The aromaticity of this compound in both the neutral and protonated form will be discussed in detail based on experimental results and theoretical analysis.References[1] J. L. Sessler and D. Seidel, *Angew. Chem. Int. Ed.*, 2003, 42, 5134.[2] H. Mori, J. Lim, D. Kim and A. Osuka, *Angew. Chem. Int. Ed.*, 2013, 52, 12997.

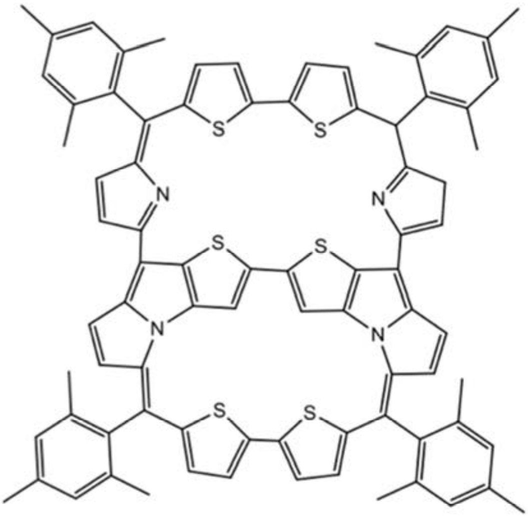

Figure 1. Chemical structure of the doubly N-fused bithiophene-bridged octaphyrin.

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Coordinative Amphiphilic siRNA Transporters

한정화 신서연[1] 백두종 금교창[2] 방은경[3,*]

상명대학교 화학과 [1]경희대학교 화학과 [2]한국과학기술연구원(KIST) 케모인포메틱스연구센터 [3]한국과학기술연구원(KIST) 뇌의약연구단

RNA interference (RNAi), first reported in 1998, is currently the most efficient method for gene down-regulation. The poor membrane permeability of small interfering RNAs (siRNAs) remains a hurdle, however, affecting their clinical applications as RNAi agents. Of the many reported delivery systems for siRNAs, cationic amphiphiles were the earliest to be described and remain the most popular for increasing the cellular uptake of oligonucleotides.1 Conventional cationic amphiphiles typically comprise a cationic head, a linker, and a hydrophobic tail. Electrostatic interactions between the heads of cationic lipids and the anionic phosphate backbones of siRNAs lead to their strong binding. In addition, the cationic character enhances cellular uptake of the siRNAs because the resulting cationic surfaces of the complexes have greater membrane affinity. In this talk, we discuss about coordinative-amphiphiles for use as novel siRNA transporters. As a modification of a conventional cationic lipid structure, we replaced the cationic head with zinc(II)-dipicolylamine complex (Zn/DPA) as a phosphate-directing group, and used various membrane-directing groups in the place of the hydrophobic tails.2 Unlike the electrostatic interactions of cationic amphiphiles, the siRNA binding of our amphiphiles occurs through coordinative bonds. Accordingly, we call them “coordinative amphiphiles (CAs)”. When linked with various chromophores, Zn/DPA has been studied widely for its ability to recognize phosphate ions.3 In this case, the Zn/DPA head groups bind to the phosphate backbones of siRNAs, and to our surprise, they prevented the enzymatic degradation of siRNAs by RNase A. Interestingly, the Zn/DPA head itself exhibited moderate transfection efficiency, and its combination with various membrane-directing groups enhanced the delivery efficiency without imparting significant cytotoxicity. Thus, it appears possible to develop tunable siRNA transporters simply by changing the membrane-directing parts. These are the first examples of amphiphilic siRNA transporters accompanying coordinative interactions between the amphiphiles and siRNAs. References1. a) . Nayerossadat, N., Maedeh, T., Ali, P. A. Adv. Biomed. Res. 2012, 1, 27–37. b) Kanasty, R., Dorkin, J. R., Vegas, A., Anderson, D. Nat. Mater. 2013, 12, 967–977.2.Kim, J. B.; Lee, Y. M.; Ryu, J.; Lee, E.; Kim, W. J.; Keum, G.; Bang, E.-K., Bioconjugate Chem. 2016, 27, 1850–1856.3. a) Sakamoto, T., Ojida, A., Hamachi, I. Chem. Commun. 2009, 45, 141–152. b) Ngo, H. T., Liu, X., Jolliffe, K. A. Chem. Soc. Rev. 2012,41, 4928–4965. c) Lee, S., Yuen, K. K. Y., Jolliffe, K. A., Yoon, J. Chem. Soc. Rev. 2015, 44, 1749–1762.

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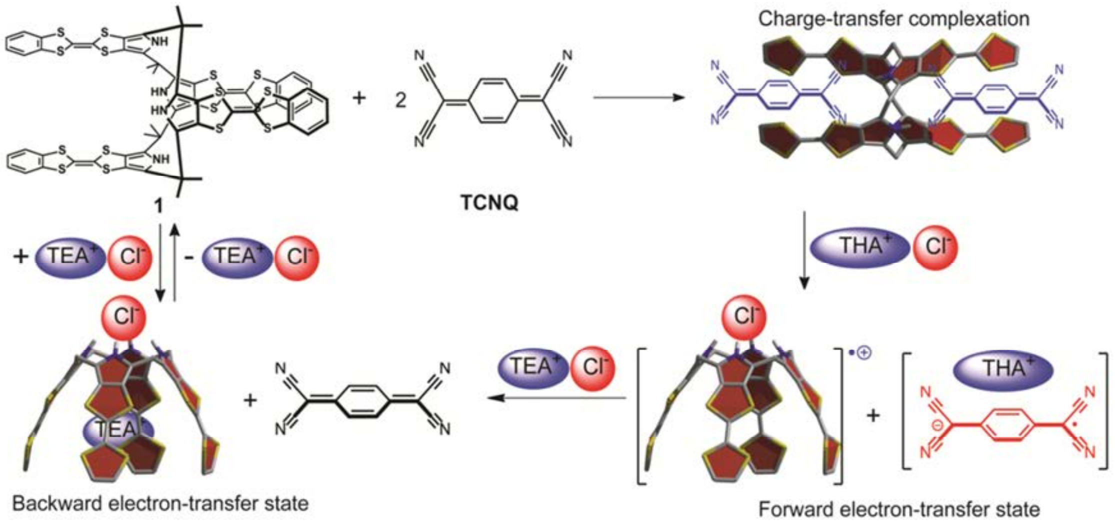
Ion Controlling Switchable Electron- and Charge-transfer Process Between Benzo-TTF-Calix[4]pyrrole and TCNQ

양윤재 박정수*

숙명여자대학교 화학과

Controlling electron- and charge-transfer processes in terms of the direction and magnitude is ubiquitous and play critical roles in a wide range of artificial and biological energy systems. These processes have also provided testbeds for theory and serves as a basic platform for operating various types of electronic materials. Until this late day, the main approach to controlling electron flow in the artificial redox systems has been an appropriate combination of two redox partners based on the exergonicity[1]. Here, we report a switchable electron- and charge-transfer process that relies on different and readily controllable interactions between an electron rich TTF-based macrocycle, benzo-tetrathiafulvalene-calix[4]pyrrole (Benzo-TTF-C4P), and an electron deficient partner, 7,7,8,8-tetracyanoquinodimethane (TCNQ). Such control is achieved by the selective inputs of tetraalkylammonium halide salts. The state-to-state switching processes have been characterized by X-ray crystallographic analyses, as well as various solution phase methods, including UV-Vis-NIR, EPR, and NMR spectroscopies.Reference[1] A. Jana, M. Ishida, J.S. Park, S. Bahring, J.O. Jeppesen, and J.L. Sessler, *Chem. Rev.*, ASAP. DOI: 10.1021/acs.chemrev.6b00375



Scheme 1. Schematic representation of ion-controlled charge- and electron-transfer processes observed using an electron rich receptor, Benzo-TTF-calix[4]pyrrole **1**, and a TCNQ acceptor.

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발표코드: **ORGN.P-381**
발표분야: 유기화학
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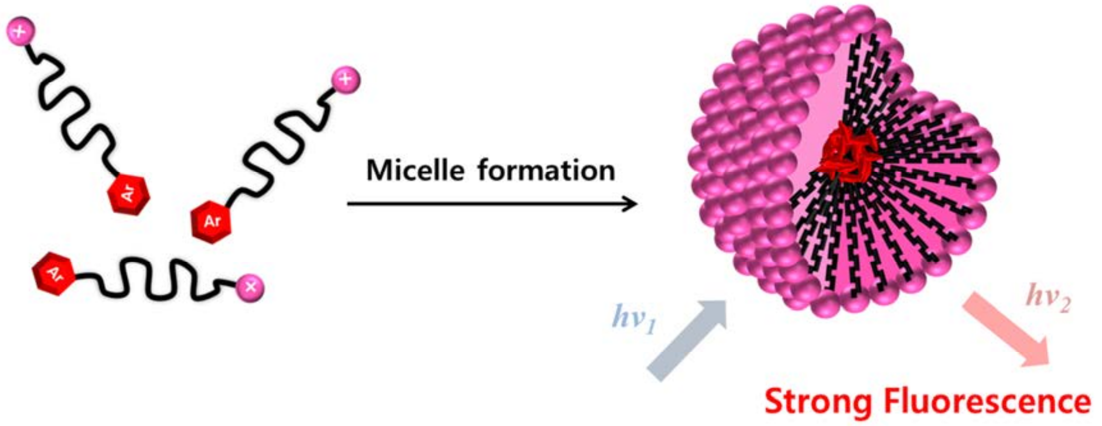
Photophysics and Energy Transport in Conjugated Polyelectrolyte Micelles

김보연 장연진 이성호*

대구대학교 화학응용화학과

A series of amphiphilic fluorogenic system, conjugated polyelectrolyte micelles (CPMs), have been newly designed and characterized. These systems contain an ionic side group and an aromatic moiety on each side of the alkyl chain, giving the conjugated polyelectrolyte micelle (CPM) formation in aqueous solution. The photophysical properties of the series of CPMs were investigated in CH3OH and H2O solutions by absorption and stead-state fluorescence. The π-extended conjugated system in CPM allows enhanced optical properties, resulting in efficient energy or electron transfer, and high quantum yield.



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장소: 일산 KINTEX
발표코드: **ORGN.P-382**
발표분야: 유기화학
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An Efficient Protocol for the Synthesis of Clickable Amphiphilic Molecules from Functionalized Polyethylene Glycol- Lignoceric Acid

박수홍 강석민 Mdabutaher 김명웅* 김동욱*

인하대학교 화학과

We have synthesized functionalized amphiphilic molecules using lignoceric acid and polyethylene glycol (PEG) bonded azadibenzocyclooctyne (ADIBO). The obtained product was determined by proton NMR and fast atom bombardment (FAB) mass spectroscopy. The resultant amphiphilic molecules are able to react with organic azide compound through strain-promoted alkyene-azide cycloaddition (SPAAC) which is highly efficient process compared Copper-catalyzed azide–alkyne cycloaddition (CuAAC). The signatures of this amphiphilic molecules synthesis protocol are avoidance catalyst, providing good yield, and no column chromatography.

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Bis-Oligoethylene-Glycol-Bridged-Calix[4]arene as Multifunctional Promoter in SN2 Fluorination

한혜지 변강록 우상식 **Mudumala Veeranarayana Reddy** 김동욱*

인하대학교 화학과

A bis-tert-alcohol-functionalized crown-6-calix[4]arene (BACCA) was studied as multifunctional organic promoters. As using BACCA, we obtained consequence that BACCA was effectively promoter Due to the fact that Cs+ was bound to crown-6-calix[4]arene, CsF with release of free fluoride. Through this reaction, we designed bis-oligoethylene-glycol-bridged-calix[4]arene and controled various ring size based on BACCA that is expected as multifuctional promoter in SN2 fluorination.

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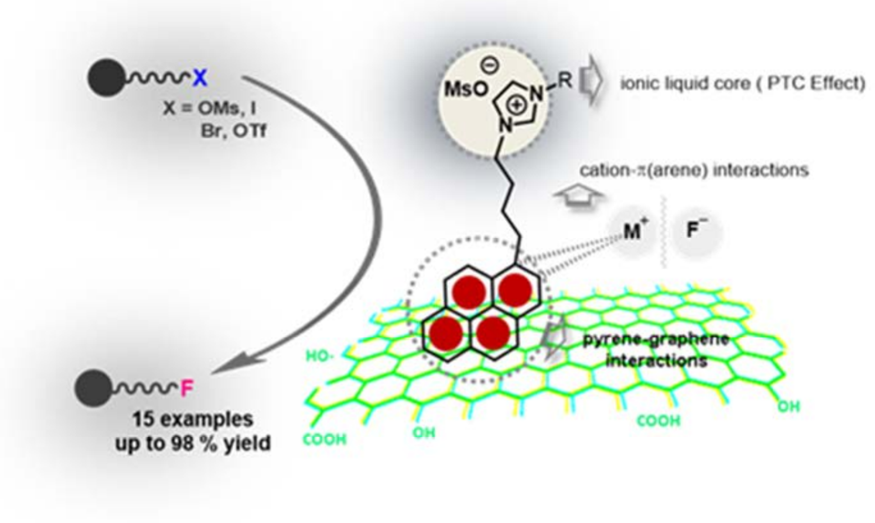
Pyrene-tagged ionic liquid frameworks: An efficient organocatalyst for nucleophilic fluorination of various substrates

Mdabutaher 강석민 박수홍 김동욱*

인하대학교 화학과

Highly efficient, easily separable pyrene-tagged ionic liquids (PTILs) were designed and synthesized as metal-free organocatalyst for nucleophilic fluorination of various substrates. The catalytic efficiency of the PTILs as phase transfer catalysts (PTCs) were demonstrated by the high conversion of the reactants using the corresponding metal fluorides (MFs) in CH3CN or t-amyl-OH. Further investigation of these findings led to the discovery of new strategy, which show superior catalyst separation process, i.e., catalyst is effortlessly separated from the reaction mixture using reduced graphene oxide (rGO). Importantly, the catalyst not only enhances the reactivity of bimolecular nucleophilic substitutions (SN2) within a short reaction time and reduces the formation of by-products but also affords high yield with easy isolation and separation under mild conditions.


X = OMs, I
Br, OTf
F
15 examples
up to 98 % yield
MsO
N
N
R
ionic liquid core (PTC Effect)
cation-π(arene) interactions
M+
F−
pyrene-graphene
interactions
HO-
OH
COOH
COOH
OH

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발표분야: 유기화학
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Ultrasensitive detection of 3,5-dinitrosalicylic acid by conformationally rigid pyreneamide dipode

Ashwani Kumar 채필석[1,*]

한양대학교 바이오나노학과 [1]한양대학교 생명나노공학과

Salicylic acid (SA), known for its ability to relief pains and aches has been widely used as an anti-inflammatory drug. Recently, SA and its derivatives were also used in many medicinal products. In addition, SA has been used in shampoos to treat dandruff.1 Based on the utility of 3,5-dinitrosalicylic acid (3,5-DNSA) in various biological studies,2 we designed and synthesized conformationally rigid or flexible pyrene-appended dipodal probe (probe 1 or 2) for selective and sensitive detection of this aromatic carboxylic acid (DNSA) in aqueous solution. These probes (probes 1 and 2) showed fluorescence quenching upon DNSA binding, with a limit of detection (LOD) of 3 and 1 nM, respectively. The fluorescence emission of a control probe (probe 3) with one pyrene unit was also “switched off” upon interaction with DNSA, but with a reduced sensitivity. The interactions of DNSA with probes 1-3 were examined by UV-visible, fluorescence, and 1H NMR spectroscopy and were supported by DFT calculations. A very low LOD (1 nM) for DNSA sensing was obtained from the use of a probe 1-coated paper strip.

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Synthesis and Self-Assembly of Adamantane-Containing Amphiphilic Block Copolymers

손창국 양시경*

전남대학교 화학교육과

Poly(norbornene)-based block copolymers containing side chains of adamantane/tetraethylene glycol (TEG) monomethyl ether or adamantane/n-butyl groups were synthesized. The adamantane- and TEG-functionalized AB block copolymer is amphiphilic enough to form micelles in aqueous media. In contrast, the other polymer is not amphiphilic because both adamantane and n-butyl side chains are hydrophobic. However, upon addition of β-cyclodextrin (β-CD), the hydrophobic adamantane side chains are decorated with hydrophilic β-CDs through host-guest interactions, affording amphiphilic AB block copolymers that can be self-assembled into micellar structures. The polymeric micelles obtained using the two different approaches in this study can also be disassembled through competitive host or guest molecules. The self-assembly and disassembly processes are characterized by TEM and SEM images.

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Synthesis and characterization of new near-infrared fluorescent glucose tracer for glucose uptake monitoring in live cell condition

조아라 성준[1] 박승범 김은하[1,*]

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Glucose plays many important roles in our body and is major source of energy as well as components of cell membrane. The imbalance of glucose homeostasis is the key feature of various diseases such as cancer, diabetes and obesity. Therefore, glucose uptake monitoring tracers have drawn significant research attention as diagnostics tools and to develop screening system for discovery of novel therapeutic agents to treat metabolic diseases. On the other hand, near infrared (NIR) region has many advantage for fluorescent live cell imaging. For these reasons, we developed new NIR fluorescent glucose tracer utilizing silicon rhodamine fluorophore to make suitable bioprobe for glucose uptake monitoring in live cell condition. The detailed results will be discussed in the poster section.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ORGN.P-388**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

반응성 조절 전략을 통한 다양한 퀴나졸린 유도체의 합성

이재빈 홍성유[1,*] 강미은

UNIST 화학공학부 [1]UNIST 나노생명화학공학부

반응성 조절을 통한 단일 물질의 다양화는 현대의 유기합성에 있어 아주 중요한 문제로 대두되고 있다. 이에 따라 우리는 반응성 조절을 통해 의학적으로 유용한 물질인 퀴나졸린 유도체를 다양화 시키는데 성공하였다. 전이 금속을 이용하거나 혹은 특별한 시약을 사용하여 반응성이 낮다고 알려진 탄소 수소 결합 등을 활성화 시키는데 성공하였다. 이 반응은 특히, 특별한 비활성 기체의 사용 없이 일반 대기 상태에서 반응이 진행되며 그 수득률 또한 아주 높다는데 그 의의가 있다. 마지막으로, 이 합성 물질의 의학적 가능성 역시 고려 해 볼만한 결과가 나왔다는 사실 또한 의미가 있다고 할 수 있다.

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Synthesis and Analysis of Mild Energetic Plasticizer for PBX

전영진 권국태[1] 김승희[2] 이소정[3] 추초롱[4] 김진석[1,*]

과학기술연합대학원대학교(UST) 무기체계공학 [1]국방과학연구소 4본부 2부 [2]국방과학연구소 4본부2부 [3]국방과학연구소 4-2 [4]국방과학연구소 4본부

PBX are mainly composed of explosives, binders, and plasticizers, etc. Polymer binders give dimensional stability and insensitivity to compound explosives. And Plasticizers provide workability, insensitivity and physical properties when processing PBX and charging it into the body. Major plasticizers are adipate plasticizers such as DOA (Dioctyl Adipate), DEHA (Bix (2-ethylhexyl) Adipate) and phthalate plasticizers such as DIBP (Diisobutyl Phthalate). However, these plasticizers have a low energy due to their simple structure, and they have a disadvantage that the performance of the PBX decreases as much as the plasticizer content.As an effort to overcome this problem, many researches on energizing plasticizers that introduce nitrate, nitro, or azide groups into plasticizers have been carried out in the same way as explosive. The performance of such energy plasticizers is improved as predicted but is very sensitive and limited to explosive. In this study, cyclic ester was synthesized by using cyclobutane as a basic energy structure to induce energy increase by adding cyclic stress to the plasticizer, and energetic functional groups were introduced into both branches. And the properties of derivatives were compared with that of the DOA with the same number of carbon atoms.

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발표코드: **ORGN.P-390**

발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Adoptation of Geometry on Anion Binding of Benzimidazole-Picket Calix[4]pyrrole

이창희* <u>bezaendalemulugeta</u> Ranjan Dutta

강원대학교 화학과

The anion recognition chemistry of calix[4]pyrroles has been actively studied due to the ubiquitous role of anions in many chemical and biological processes. As a result, various systems have been developed in order to improve the affinity and selectivity toward anion. Among various reported 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, we report the anion recognition properties of the a deep cavity calix[4]pyrrole derivatives carrying 5,6-dichlorobenzimidazole units at diametrically crossing meso-positions. The receptor shows high affinity for anions especially for chloride and fluoride anion. The additional hydrogen bond donors placed on the picket component are attributed to the enhancement of the binding affinity. The cooperative interaction of anion-pi interaction and hydrogen bond are thought to be the reason for exceptionally high binding affinity. However, the fluoride anion forms six-point hydrogen bonding complex with host molecule while chloride anion forms four-point hydrogen bonding complex. This size-dependent changes in binding mode indicates that the synthesized receptor is capable of molecular level adaptation. The detailed guest binding studies obtained from 1H NMR titration and ITC will be presented in detail.

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Dicationic meso-bis(Benzimidazolium) Calix[4]pyrrole as Recognition, Sensing and Bicarbonate Anion Activation Motif

이창희* <u>bezaendalemulugeta</u> Divya Sareen[1] Qing He[2] Jonathan Sessler[2] 김성국[3]

강원대학교 화학과 [1]Guru Nanak Dev University [2]University of Texas at Austin [3]경상대학교 화학과

Calix[4]pyrroles carrying cationic benzimidazolium or benzimidazole units at diametrically crossing meso-positions have been synthesized and fully characterized. The synthesis was accomplished by '2+2' type condensation of meso-[(2-benzimidazoly)-methyl]dipyrromethane and acetone in the presence of acid catalyst. The synthesized receptor displays strong affinity toward various anions with slow complexation/decomplexation kinetics. Similar binding behavior was observed with other dicationic analogues, but current receptor displayed exceptionally high selectivity toward bicarbonate anion. The cooperative effects of hydrogen bonding, Coulombic interaction and anion-pi interactions were attributed to the exceptionally high binding affinity. The receptor acts an effective host for the bicarbonate anion at concentrations as low as 4.1 nM. A change in fluorescence response was observed under conditions of fluorescence dye displacement when this functionalized calix[4]pyrrole is exposed to the HCO3– anion. Tests with various carbonated drinks revealed its ability to function as an easy-to-use sensor for dissolved CO2 as monitored through bicarbonate anion concentration.

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Synthesis, Structure and Spectroscopic Properties of Difluoroboron Dipyrromethene Complexes of Carbazole-Benzimidazole Conjugates

이창희[*] <u>Ranjan Dutta</u> Firmansyah DIKHI

강원대학교 화학과

Boron dipyrromethene (BODIPY) derivatives are widely used as biomolecule markers, fluorescent switches, chemosensors and laser dyes. Remarkable versatility of BODIPYs has sparked intense research on new modification strategies to enable their attachment to biological substrates and also to tune their optical properties. On the other hand, 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. A series of carbazole-benzimidazole conjugates and their BODIPY complexes are synthesized and their spectroscopic properties are investigated. Benzimidazole, N-alkyl benzimidazole, N-phenyl benzimidazole substituents were introduced at the 1-position of the carbazole moiety and boron complexation of each dipyrrin generated the corresponding BODIPYs. X-ray crystal structures of two complexes unambiguously confirmed the BODIPY skeletons. 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.

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Synthesis and Properties of Annulated, Planar Hexapyrrolic Macrocycles

이창희* **Firmansyah DIKHI** 고유림

강원대학교 화학과

Two novel annulated rosarins were synthesized, their synthetic procedure and properties are presented. Annulated rosarin or o-phenylene bridged rosarin (hexaphyrin 1.0.1.0.1.0) is an antiaromatic 24 π-electrons molecule with unique redox behavior. While typical protonation on hexaphyrins gave only triprotonated species, annulated rosarin can form triprotonated, non-aromatic 25 π-electrons, or aromatic 26 π-electrons species depending on the acid. We introduced two differents electron deficient groups on the rosarin periphery to further study their aromaticity behaviors. The first compound was obtained by complexation of rosarin with boron trifluoride in the presence of an amine and the second rosarin was prepared from an imide substituted naphthobipyrrole building block. Proton NMR and Mass spectra clearly indicates the formation of one boron complex inside rosarin cavity. Stability of the boron complex was investigated and their unique protonation behaviors were studied.

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Control of Fries Rearrangement within Microseconds to Milliseconds Using Microfluidic Devices

김희진 김동표[1,*] **Jun-ichi Yoshida**[2,*]

Kyoto University 공학연구과 합성화학전공 [1]POSTECH 화학공학과 [2]Kyoto University, Japan

A micro- or milli-second timescale is barely perceptible in our life, but it sometimes can be essential for the control of fast chemical reactions. For example, intramolecular chemical reactions sometimes too fast even at very low temperature to control to proceed or not in accordance with our synthetic purpose. In these case, the controllability of micro- to milliseconds is crucial for the achievement of desired chemical reactions. Herein we report flow-assisted rearrangement control of anionic Fries rearrangements via microfluidic devices. Although several intramolecular rearrangements were too fast to control even at very low temperature using a flask, flow microreactors served as a good method to control these rapid transformations via the control of submilliseconds timescale. This methodology was successfully applied to the synthesis of biologically active compound.

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Development of Complex Peptoid Structures

김수민 송지현 임현주 권용억*

이화여자대학교 화학.나노과학과

Peptides are well known to be fascinating chemical tools for chemical biology and drug development. However, they are sensitive to proteolytic degradation and exhibit a limited cell permeability and a poor bioavailability in many cases. Thus, various peptidomimetics-based chemical tools have been developed to overcome these drawbacks. Among them, peptoids, N-alkylated oligoglycines possess many advantages in terms of physico-chemical and pharmacological properties over peptides. Generally, many people tend to believe that cyclic molecules may bind to their target proteins with higher affinity because of their limited conformational flexibility. In addition, cyclic peptoids might possess an enhanced cell permeability and an improved resistance to enzymatic degradation. Thus, they have been synthesized by several different chemical methods. However, complex peptoid structures in three-dimension which may be more rigid and unique are presumed to be much more useful as chemical tools or molecular probes but not yet developed. Therefore, we have tried to develop various complex peptoids including bridged forms. In this presentation, we will introduce our efforts on the synthesis of sandwich-type peptoid structures via macrocyclization followed by click reaction.

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Controlled Growth of Amyloid Fibrils on Patterned Self-Assembled Monolayers

신재호 송하은 강경태*

경희대학교 응용화학과

Despite a large amount of previous efforts and huge interest in neurological diseases such as Alzheimer's disease and Parkinson's disease, the exact cause of neurological diseases is unknown except some contradicting hypotheses. One important issue is to understand the aggregation process of amyloid fibers, the main component of amyloid plaques. The aggregation contains numerous temporally existing amyloid species that assemble in a non-equilibrium fashion, which makes it extremely hard to understand. As a fresh direction to approach to understand the aggregation process, we introduced a micro patterned gold substrate as a model system with which to generate controllable amyloid fibrils. For making patterns, we used OH-terminated and COOH-terminated alkanethiols for assembling them on gold substrates in a mixed ratio. The dimension and geometry of the micropatterns dictated the formation of amyloid fibers grown on top. By varying the dimention of the micropattern, the type of the amyloid-forming proteins, and aggregation conditions we could obtain amyloid fibers with different physical properties (e.g., dimension, morphology, and migratory abilities), which provided indirect information about their aggregation kinetics. We expect that our approach can suggest a novel and straightforward model system to study fundamentals of amyloid aggregation processes.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ORGN.P-397**

발표분야: 유기화학

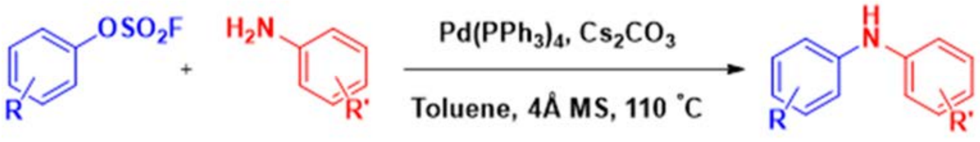
발표종류: 포스터, 발표일시: 목 11:00~12:30

Palladium-catalyzed, Buchwald-Hartwig 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 with the use of palladium catalysts with an array of ligands.1 Aryl fluorosulfonates can be prepared in quantitative yields from the reaction of phenol derivatives and sulfuryl fluoride, and we tested if aryl fluorosulfonates could be applied as alternative cross-coupling partners to aryl halides in palladium-catalyzed aminations.2 We report the direct amination of aryl fluorosulfonates with arylamines using Pd(0) catalysts. This Buchwald-Hartwig type amination occurs under mild conditions in the presence of Pd(PPh3)4, without any additional N- or P-type ligand. This protocol provides a quite straightforward alternative for the amination of aryl amines, using aryl sulfonates instead of aryl halides.Reference1.John P. Wolfe and Stephen L. Buchwald, J. Org. Chem. 1997, 62, 1264-12672.Qiaobin Liang, Ping Xing, Zuogang Huang, Jiajia Dong, K. Barry Sharpless, Xiaoxian Li, and Biao Jiang, Org. Lett. 2015, 17, 1942−1945



ligand-free conditions, 20 examples

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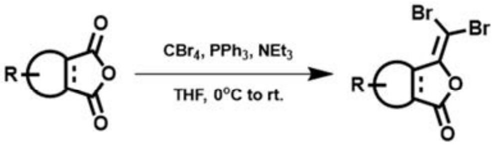
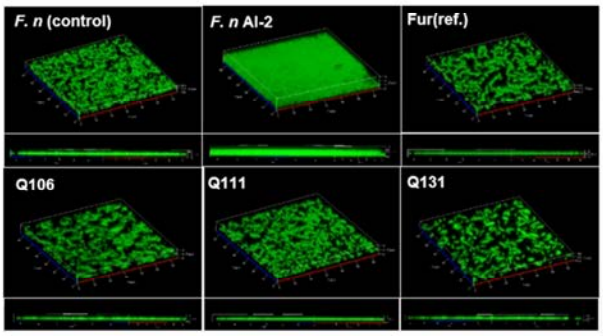
New bicyclic brominated furanones: Potent autoinducer-2 quorum sensing inhibitors against periodontal biofilm formation

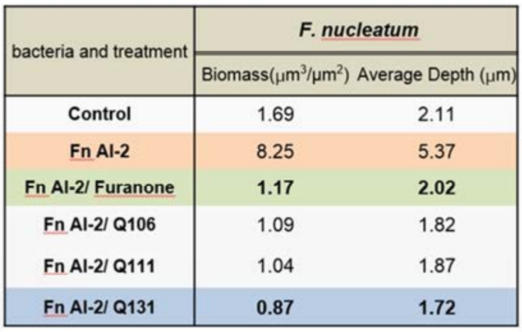
박지수 김병문*

서울대학교 화학부

Bacterial behaviors, including virulence factor expression, bioluminescence, and biofilm formation, are effectively regulated through quorum sensing, a mechanism of intra- and interspecies communication in response to changes in cell density through recognition of the threshold reached by autoinducers. Among these bacterial behaviors, formation of a biofilm can be the basis of the development of chronic inflammatory diseases. Periodontitis, a chronic inflammatory disease affecting the periodontium, is caused by subgingival biofilms related to periodontopathogens. In particular, Fusobacterium nucleatum is known as a major co-aggregation bridge organism that connects early commensal colonizers and late pathogenic colonizers in periodontal biofilms. According to a previous study, the intergeneric quorum sensing signal molecule autoinducer-2 (AI-2) of F. nucleatum plays a key role in intra- and interspecies interactions of periodontopathogens, and may be a good target for periodontal biofilm inhibition. Recently, brominated furanones produced by the macroalga Delisea pulchra were shown to inhibit biofilm formation, and have been investigated toward the goal of increasing the inhibition effect. In this study, to improve the antagonistic activity and better understand structure-activity relationship, we describe the synthesis of new brominated furanone analogs, i.e., 3-(dibromomethylene)isobenzofuran-1(3H)-one derivatives, and demonstrate their inhibitory activities against biofilm formation by periodontopathogens.







bacteria and treatment	*F. nucleatum*	
	Biomass($\mu m^3/\mu m^2$)	Average Depth (μm)
Control	1.69	2.11
Fn AI-2	8.25	5.37
Fn AI-2/ Furanone	**1.17**	**2.02**
Fn AI-2/ Q106	1.09	1.82
Fn AI-2/ Q111	1.04	1.87
Fn AI-2/ Q131	**0.87**	**1.72**

- ***F. n*** : *F. nucleatum* (ATCC 25586)
- ***F. n* AI-2** : *F. nucleatum* + *F. nucleatum* AI-2
- **Fur** : *F. nucleatum* + *F. nucleatum* AI-2 + furanone compound 2 μM
- **Q series** : *F. nucleatum* + *F. nucleatum* AI-2 + BMK-Q series compounds 2 μM

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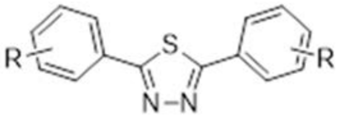
Synthesis of 2,5-Disubstituted-1,3,4-Thiadiazoles and Its Biological Evaluation

박수진 김학원[1,*] 오혜리[1] 신호철[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 various 1,3,4-thiadiazoles via Suzuki coupling with bromophenyl derivatives or demethylation of methoxyphenyl derivatives. Newly synthesized 2,5-disubstituted-1,3,4-thiadiazole derivatives were tested to biological activities such as anti-virus, anti-inflammatory and other pharmacological activities.



2,5-Disubstituted-
1,3,4-thiadiazole

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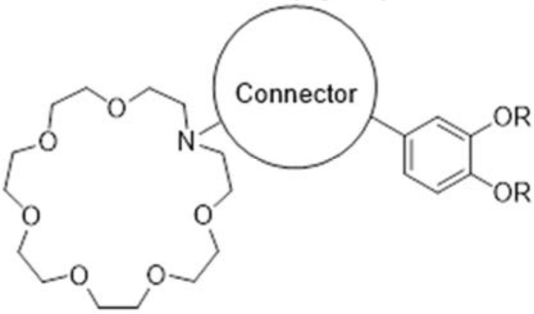
장소: 일산 KINTEX
발표코드: **ORGN.P-400**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel CO_2-Soluble Aza-21-crown-7 Ethers for the Metal Extraction in Supercritical CO_2

김유로 박예슬[1] 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

In this work, we have designed and synthesized several catechol-containing aza-21-crown-7 ethers and tested their CO_2-solubility. Simple catechol-containing aza-21-crown-7 ethers were not soluble in CO_2. Thus, some CO_2-philic groups were introduced to increase CO_2-solubility and the relationship between structure and CO_2-solubility has been studied. The $scCO_2$ metal extraction has been investigated with this chelating ligand.



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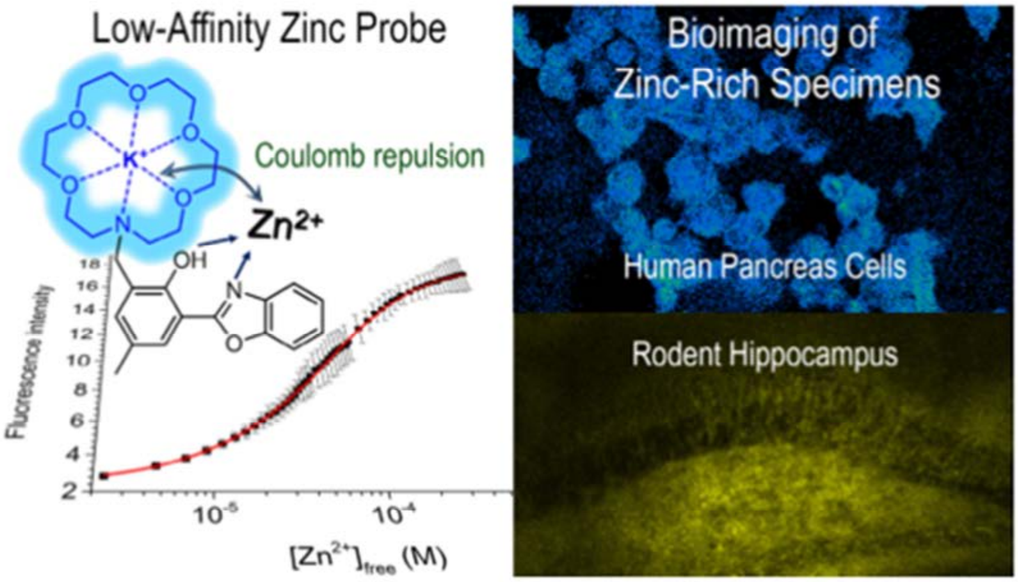
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design, synthesis, and zinc sensing properties of a novel fluorescence zinc sensor, HBO-ACR

yan xinhao 김학원[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Study of the zinc biology requires molecular probes of suitably tailored zinc affinity. We have demonstrated that the incorporation of an azacrown ether unit into an excited-state intramolecular proton-transfer (ESIPT) fluorophore can provide an effective strategy for creating a low-affinity zinc probe (2-(2-hydroxyphenyl)benzoxazole including aza-18-crown-6 ether moiety,HBO-ACR).This synthetic modification enables fluorescence turn-on responses to zinc ions without being affected by the presence of other transition metal ions, including cadmium. The probe retains its ability for fluorescence turn-on zinc detection in broad pH ranges.Steady-state and transient photophysical measurements suggest that orchestrated actions of proton-induced nonradiative and zinc-induced radiative control are operative for the high pH tolerance. Zinc bioimaging utility of HBO-ACR has been fully demonstrated with the use of human pancreas epidermoid carcinoma, PANC-1 cells and hippocampal slices collected from the brain of mice.


Low-Affinity Zinc Probe
Coulomb repulsion
K^+
O
N
OH
Zn^{2+}
Fluorescence intensity
2
4
6
8
10
12
14
16
18
10^{-5}
10^{-4}
$[Zn^{2+}]_{free}$ (M)
Bioimaging of Zinc-Rich Specimens
Human Pancreas Cells
Rodent Hippocampus

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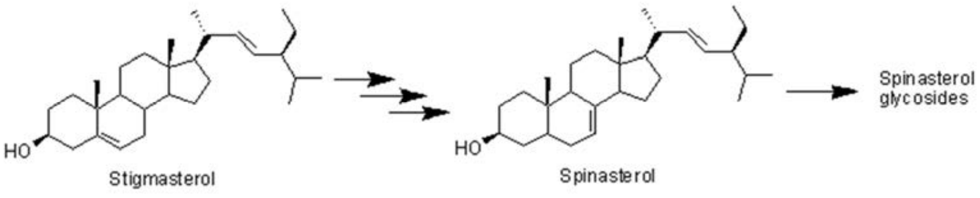
발표코드: **ORGN.P-402**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of spinasterol glycosides and its biological evaluation

조영경 고인석[1] 이태훈 김학원*

경희대학교 응용화학과 [1]경희대학교 화학과

Natural spinasterol-glucose (3-O-β-D-glucopyranosylspinasterol), isolated from *Stewartia koreana* leaves, has been identified as a compound to exhibit a potent anti-inflammatory activity. However, further biological investigation such as anti-ischemic stroke with a spinasterol glucose has not been done, because the isolation of natural spinasterol and spinasterol glucose is very difficult and inefficient. In order to study on the anti-ischemic stroke activities of spinasterol glucose and its derivatives. In the present study that spinasterol glycosides significantly attenuated expression of TNF-a induced vascular adhesion molecules-1 (VCAM-1) in human endothelial cells. These results suggest that spinasterol glycosides maybe a potent target for anti-ischemic drug candidate involving down-regulation of cells adhesion molecules in microvascular systems.



대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX

발표코드: **ORGN.P-403**

발표분야: 유기화학

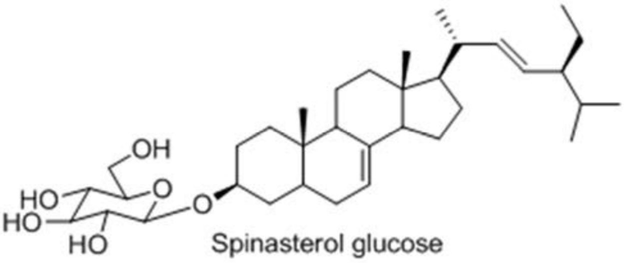
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Novel glycosyl steroids and their biological evaluation

이현진 박훈규[1] 김학원[2,*]

경희대학교 응용과학대학 응용화학과 [1]경희대학교 화학과 [2]경희대학교 응용화학과

Natural spinasterol-glucose (3-O-β-D-glucopyanosylspinasterol), isolated from *Stewartia koreana* leaves, has been identified as a compound to exhibit potent anti-inflammatory activity. However, isolation and synthesis of spinasterol and spinasterol glucose is very difficult and inefficient. To overcome these problems, we had already suggested synthetic stellasterol glycosides for the alternative of a natural spinasterol glucoses. Recently, we have found a new sterol, such as ergostenol, which can be synthesized more easily than stellasterol. In this report, a synthesis and anti-inflammatory activities of ergostenol were investigated in TNF-a/IFN-r stimulated human keratinocyte.



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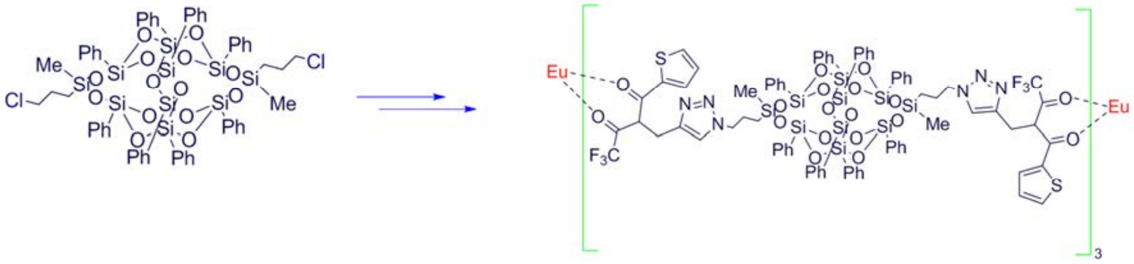
발표종류: 포스터, 발표일시: 목 11:00~12:30

Design and synthesis of photo-luminescence property material from Eu3+ ion complexing with theonyltrifluoroacetone functionalized DDSQ

신동수* **PATILKALPESHTUMADU**

창원대학교 화학과

Now many researchers working on material which use in industry, pharmacy, medical devices, and many other useful materials for improving their activity and chemical, mechanical and thermal stability. For such development organic-inorganic hybrid material are suitable to enhance such kind of properties. One of the hybrid material is DDSQ(double decker silsesquioxne), it used to give strength to compound that improves thermal, mechanical and chemical stability in polymers. Our work focuses to improve the luminescence material stability by coupling of such hybrid material. We design and synthesis using DDSQ and Eu3+ ion complexing with theonyltrifluoroacetone as new hybrid luminescence material may potentially use in electronic devices such as display.



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다양한 촉매를 이용한 퀴나졸리논 유도체 합성

강미은 홍성유[1,*] 이재빈

UNIST 화학공학부 [1]UNIST 나노생명화학공학부

전이금속 촉매를 이용해 탄소-수소결합을 끊고 새로운 탄소-탄소결합을 만드는 반응이 많이 연구되어 왔다. 그러나 기존방법은 반응물과 유도체의 구조가 간단하여 실제 존재하는 복잡한 자연물질이나 의약 물질을 합성하는데 있어 한계가 존재했다. 그래서 최근 새로운 물질을 좀 더 빠르고 쉽게 만들기 위해 복잡한 물질을 다양화 하는 연구가 개발되기 시작했다. 우리는 다양한 촉매를 이용하여 퀴나졸리논의 다양한 유도체를 합성하였고 높은 수득률을 얻어냈다. 이에 따라 시간과 비용을 절감 할 수 있어 새로운 물질을 합성하는데 유리하며 대기중의 공기나 수분에 영향을 받지 않아 합성방법도 비교적 쉬워 다양한 응용이 가능하다.

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Pd-catalyzed synthesis of substituted triphenylenes by aromatic annulation

양현지 홍성유[1,*]

UNIST 에너지화학공학부 [1]UNIST 나노생명화학공학부

After a decade of research, developing one-step synthetic methods for selective C-H arylation is still a massive challenge for synthetic chemists. The focus of our research, had been on designing an efficient route to access tailored triphenylenes by using palladium as catalyst and cyclic iodonium salts as annulating agent. Moreover, the work was extended to application of field-effect transistor sensor for alcohol vapor detection.

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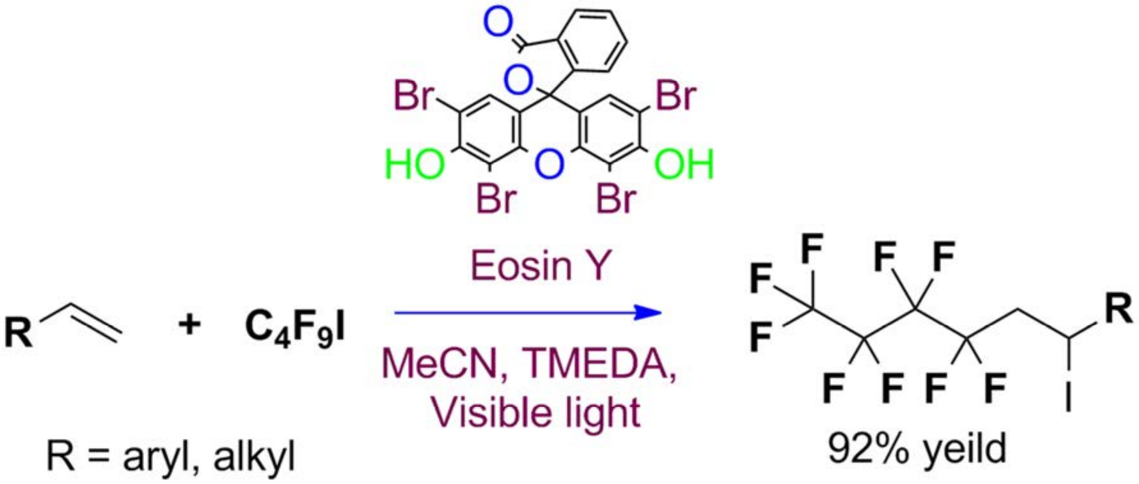
Visible light mediated perfluorination by Eosin Y

VAIDYARAGHAVENDERRAO 신동수*

창원대학교 화학과

Photocatalytic reactions have a lot of advantages like ability to control vitalities of reactions by irradiating the light, eco-friendly approach. Few decades ago scientists are used transition metal catalysts such as iridium, ruthenium, and platinum however they are expensive and could affect the efficiency of electronic materials while synthesizing it. We have been interested in eosin y because it can react mild conditions and give us high yield. Eosin y an organic dye we are using that for photo catalytic reactions it can make single electron transfers (SET) rapidly so that radicals can chain react step by step. Based on this concept we designed a new perfluorination method which is easier to handle, eco-friendly approach



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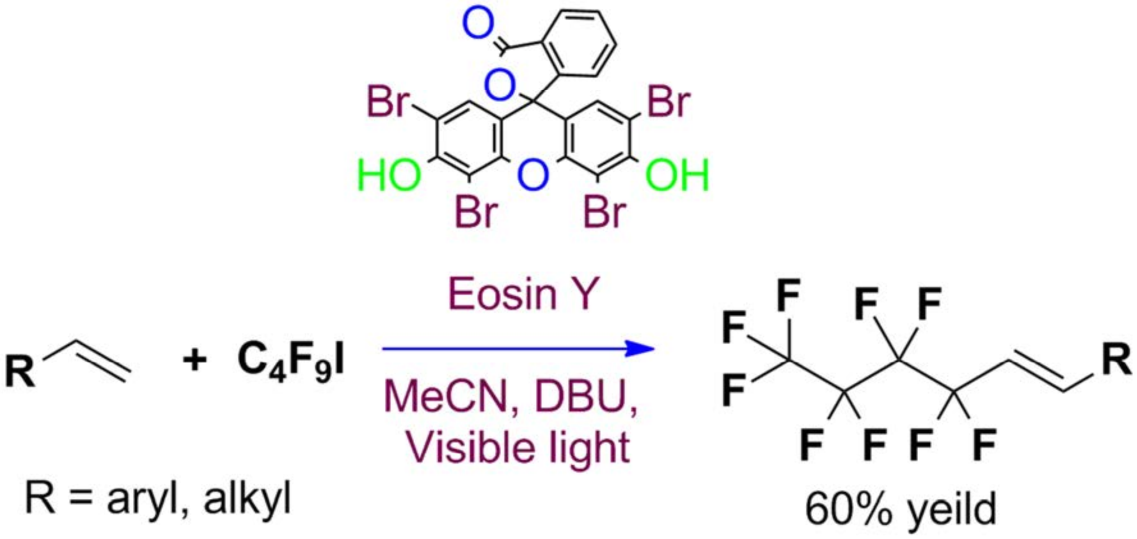
장소: 일산 KINTEX
발표코드: **ORGN.P-408**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Visible light mediated Metal-Free perfluoroalkenylation by Eosin Y

VAIDYARAGHAVENDERRAO 신동수*

창원대학교 화학과

Photocatalytic reactions have a lot of advantages like ability to control vitalities of reactions by irradiating the light, eco-friendly approach. Few decades ago scientists are used transition metal catalysts such as iridium, ruthenium, and platinum however they are expensive and could affect the efficiency of electronic materials while synthesizing it. We have been interested in eosin Y because it can react mild conditions and give us high yield. We are using that for photo catalytic reactions it can make single electron transfers (SET) rapidly so that radicals can chain react step by step. And adding DBU (Diazabicycloundecene) as a base we can get fluorinated alkene. Based on this concept we designed a new perfluorination method which is easier to handle, eco-friendly approach.



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장소: 일산 KINTEX
발표코드: **ORGN.P-409**
발표분야: 유기화학
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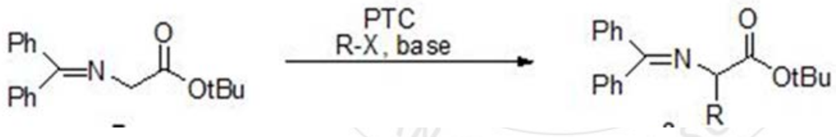
Enantioselective Dimeric Cinchona-Based Ammonium Phase Transfer Catalysts for the Synthesis of α-Amino Acids

우승아 임배근 남기평*

영남대학교 화학과

Benzophenone-Bridged dimeric Cinchonium Phase Transfer Catalysts (PTC) have been developed. The alkylation with selected alkyl halides with the PTC (0.5 ~ 1.0 mol %) shows that the PTC has very high enantioselectivity (93-98% ee, rt or 0℃) and is an efficient phase transfer catalyst for the industrial synthesis of various α-amino acids.



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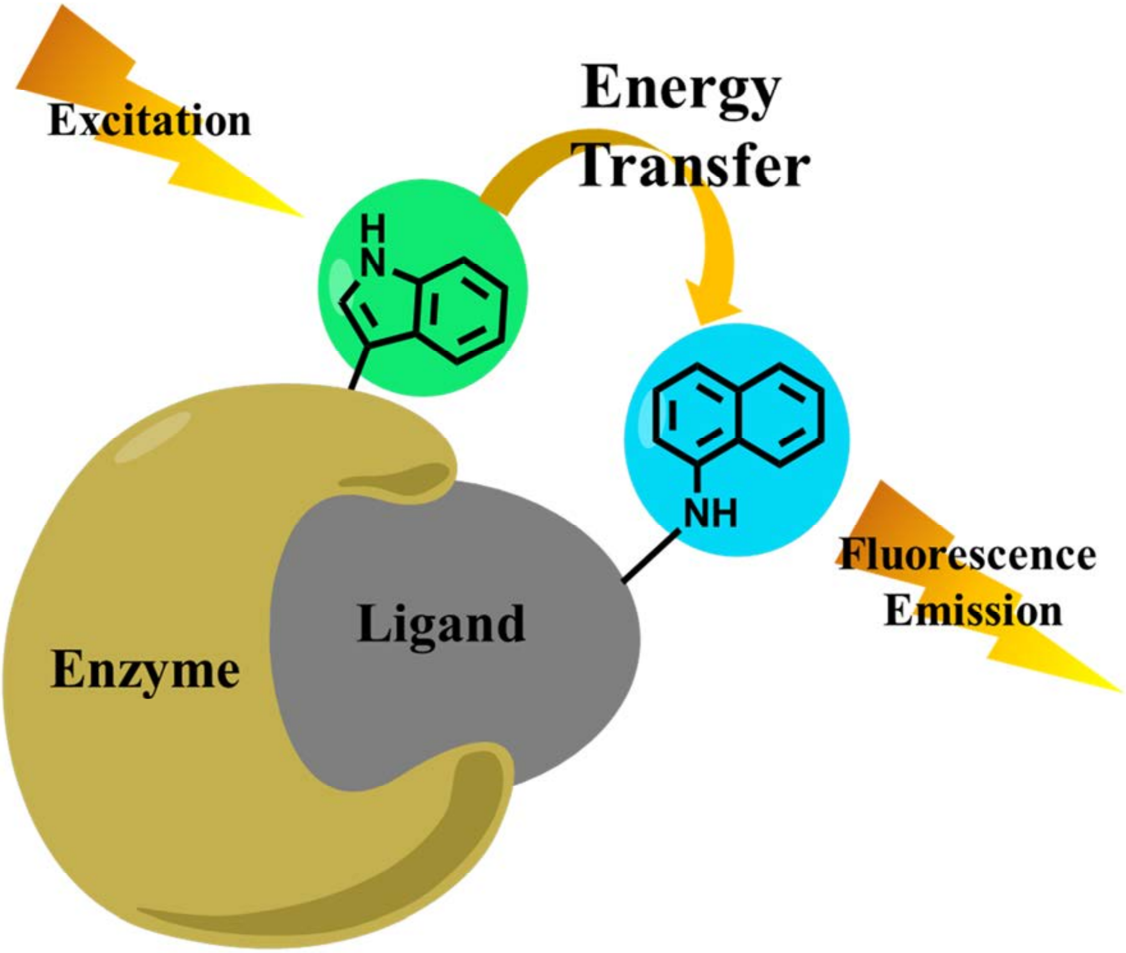
Development of a Noble Method for PAK1 Assay Applying Intrinsic Förster Resonance Energy Transfer (iFRET) Platform

나원호 정상전*

동국대학교 화학과

Kinase is an enzyme which plays a key role in cell signal transduction. PAK1, a member of kinase family, in known that causes fatal diseases such as cancer when it is overexpressed.1 Traditional kinase assays spend a myriad of expenses and time. In this study, we developed novel PAK1 assay method using intrinsic Föster Resonance Energy Transfer (iFRET) technique so that kinase assay is accomplished with low cost and saving of time. We synthesized PAK1 sensor including inhibitor moiety which can bind to ATP binding site of PAK1 and fluorophore moiety which can absorb the energy from the intrinsic tryptophan in PAK1. We confirmed the iFRET signal between the donor and the acceptor by mixing them up and measuring the emission wavelength of acceptor after excitation of the donor. This label-free PAK1 assay method is utilized for not only general inhibitor screening but also HTS with saving time and cost as much as significant. In this context, further modification of the sensor to improve iFRET signal and validation of the ability to perform in various kinase assay will be set.


Excitation
Energy Transfer
Fluorescence Emission
Enzyme
Ligand
H
N
NH

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발표코드: **ORGN.P-411**
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발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of Antibody Drug Conjugate (ADC) using Photoreactive FcBP

이태진 정상전*

동국대학교 화학과

At present, antibody drug conjugates (ADCs) is leading the field of targeted drug. The critical aspect to effective targeted drug therapies is the well-ordered release of a cytotoxic drug from the drug delivery system upon cellular internalization or localization. ADCs facilitate the internalization of their payload by taking advantage of the specificity of antibodies. Antibody is linked via stable chemical linker, a labile bond in particular condition. Stable conjugation and specific targeting result in the accumulation of high local concentrations of cytotoxic agents that would not be tolerable if administered systemically.Recently, small peptide ligands to the Fc-domain of antibodies was reported. The Fc Binding Peptide (FcBP) have high affinity to an IgG-Fc domain. The FcBP is a cyclic peptide with disulfide bond of two Cys residues and 13 amino acids. To make covalent linkage between drug and antibody, we have made photoreactive FcBP with photoreactive unnatural amino acid. Novel photoreactive FcBP is going to be conjugated with Valine-Citrulline linker containing payload and make covalent bond with antibody. This new ADC will be stable in physiological condition during transferring to target and internalize into target cells.

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발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of photo-reactive Fc binding peptide-NOTA conjugates for imaging of Rheumatoid Arthritis

이사묵 정상전*

동국대학교 화학과

Rheumatoid arthritis (RA) is a well-known autoimmune and chronic inflammatory joint disease, which can cause cartilage and bone damage as well as disability. The risk factors associated with development of RA are TNF-α, IL-1, IL-6, and IL, which are key infiltrates in inflamed subsynovium, and proinflammatory cytokines. Originally, the well-known methods for diagnosing and managing initial RA are conventional radiography, ultrasonography and magnetic resonance imaging. In our approached, we used photo-reactive Fc binding peptide and 1,4,7 triazacyclononane(TACN)based derivatives, respectively, for binding Fc domain of Envrel which is kind of antibody acted as a TNF-α inhibitor and radio isotope carrier. We have previously demonstrated that IgG Fc-binding peptide (FcBP) is a very convenient tool to link functional materials with antibodies in reversible and site-specific manner1. Furthermore, we synthesized TACN complex which have capability of strong chelating properties and higher selectivity toward di- or trivalent metal2. In our strategies, we synthesized FcBP and 1,4,7 triazacyclononane-derivatives complex covalently by photo cross linking method and conjugated with these complex and Envrel(antibody) for targeting TNF-α in our body. In addition to, we can get images of RA by scintigraphy using radio isotope. Successful development of RA diagnosing tool may find application in RA cell imaging as well as monitoring drug delivery.

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발표종류: 포스터, 발표일시: 목 11:00~12:30

Detection of protein tyrosine phosphatase 1B by intrinsic Förster resonance energy transfer

DURGANNAVAR TRISHALADEVI ASHOK 정상전*

동국대학교 화학과

Protein tyrosine phosphatase (PTP) is a family of enzymes that remove phosphate groups from phosphorylated tyrosine residues in proteins. PTPs play a key role in multiple cellular signal transduction pathways and PTP1B is implicated in many diseases. For instance, PTP1B is known to negatively regulate insulin and leptin signaling pathways. Dysregulation of insulin and leptin signaling are known to result in the development of diabetes type 2 and obesity, respectively.1 Detection PTP1B using the recently developed intrinsic Förster resonance energy transfer (iFRET) technique may be a valuable diagnostic tools in many diseases.2 iFRET is a fluorescent technique that enables real-time monitoring of protein-protein, protein-ligand interactions. Based on a difluoromethylphosphonate phenylalanine tripeptide, a known nanomolar PTP1B inhibitor, and 1-naphthyl-ethylenediamine, several iFRET acceptor probes for PTP1B were crafted using solid phase peptide synthesis protocols.3 Next, iFRET was used to evaluate the binding of the probes to PTP1B and several other PTPs. To this end, a solution of the appropriate phosphatase in the presence of the iFRET probe was excited at 280 nm, corresponding to tryptophan absorption maximum, and the fluorescence was recorded at 450 nm, corresponding to the probe emission maximum. Next, selectivity of the probes towards various PTPs and binding characteristics such as inhibition- and dissociation constants were determined. The most promising iFRET probe in terms of binding selectivity and affinity was found to be a dipeptide probe with a Kd values of about 0.1 μM and Ki 40 nM. Our developed iFRET probe may be used to build PTP sensors which can be used in the early diagnostics of diabetes type 2 and related diseases.

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Visible-light-induced aerobic oxidative coupling reaction of N-phenyl tetrahydroisoquinoline with -keto acids

김유빈 김대영*

순천향대학교 화학과

The application of visible light mediated photoredox catalysis has emerged as a novel and efficient tool for chemical transformations due to its natural abundance, mild and relatively clean reaction conditions, and high reactivity. A visible light mediated photocatalytic oxidative coupling reaction of N-phenyl tetrahydroisoquinoline with -keto acids has been developed. This approach provides a mild and operationally simple access to the synthesis of C1-phenacylmethylated tetrahydroisoquinolines.

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장소: 일산 KINTEX
발표코드: **ORGN.P-415**
발표분야: 유기화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Internal Redox reaction via[1,5]-Hydride Shift/7-Endo Cyclization Sequences : Synthesis of Ring-Fused 1-Benzazepines

권수진 김대영*

순천향대학교 화학과

Benzo-fused, seven-membered aza-heterocycles have attracted continued attention in the fields of organic and medicinal chemistry due to their importance as building blocks and because of the diverse array of their biological activities. Synthesis of 1-benzazepines has been achieved via a [1,5]-hydride shift/7-endo cyclization sequence. The focus of this research is a direct transformation of 2-(aryl)cyclopropane 1,1-diester derivatives into 1-benzazepines using a cyclopropane moiety as the hydride acceptor in internal redox reactions.

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Synthesis of Ring-Fused Tetrahydroquinoline Derivatives via [1,5]-Hydride Transfer/Cyclization Sequences

김연주 김대영*

순천향대학교 화학과

Tetrahydroquinoline derivatives have attracted considerable attention in organic and medicinal chemistry due to their importance as building blocks and broad array of biological activities. Herein, we report the synthesis of 3-nitro tetrahydroquinoline derivatives from 2-(o-(dialkylamino)aryl)nitroalkenes via [1,5]-hydride transfer/cyclization sequences.

일시: 2017년 4월 19~21일(수~금) 3일간

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발표분야: 유기화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of a Protocol for Copper-Catalyzed Enantioselective Conjugate Addition

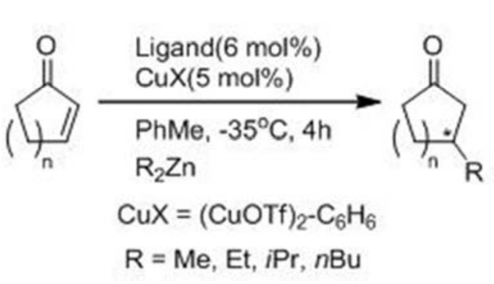
신민경 정병혁*

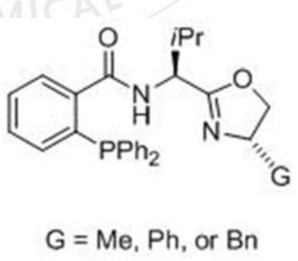
DGIST 기초학부

Reactions of forming enantioselective C–C bonds have been essential in the syntheses of various bio-active compounds. One of these reactions is the conjugate addition of organocuprate to α, β-unsaturated enones. Herein, we report our endeavors of developing enantioselective synthetic method by applying novel copper catalysts.

References

1. López, F.; Minnaard, A. J.; Feringa, B. L. *Acc. Chem. Res.* **2007**, *40*, 179-188.
2. Katsuki, T.; Sharpless, K. B. *J. Am. Chem. Soc.* **1980**, *102*, 5974.





일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-418**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

SYNTHESIS OF 1,2,3-TRIAZOLES VIA CYCLOADDITION OF β-KETOPHOSPHONATE WITH AZIDE

이두현 김다현 이태호*

경북대학교 약학과

1,2,3-Triazoles, which are non-classic bioisosteres of amides, are important heterocycles in medicinal chemistry and material science. Because of their widespread applications, a number of copper(I)-catalyzed azide-alkyne cycloaddition reactions for the preparation of 1,4-substituted 1,2,3-triazoles have been performed. However, synthetic methods for the preparation of 1,5-substituted 1,2,3-triazoles have been known as restricted. Also, these known methods have usually used limited terminal alkyne and expensive ruthenium-catalysts. Therefore, the development of new efficient methods for the preparation of 1,5-substituted 1,2,3-triazoles is still demanded. β-Ketophosphonates are well-known and important intermediate in organic synthesis. They are widely used for the synthesis of α,β -unsaturated carbonyl compounds via Horner-Wadsworth-Emmons (HWE) olefination and for the synthesis of β-amino phosphonate compounds via Mannich-type reaction, and for the synthesis of phosphonylated heterocyclic compounds. Herein, we report the general and efficient cycloaddition reaction of β-ketophosphonate with azide for the preparation of 1,5-disubstituted 1,2,3-triazoles and 1,5-disubstituted 4-phosphoryl 1,2,3-triazoles under basic conditions.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Validated high-performance liquid chromatography method for the inhibitor of cancer cell invasion in rat plasma and its application to pharmacokinetic study

최현경* 김정수

중원대학교 의약화학과

In this study, a reliable method for the quantitation of (E)-N-benzyl-6-(2-(3, 4-dihydroxy benzylidene)hydrazinyl)-N-methylpyridine-3-sulfonamide (JW-55) in rat plasma was developed and validated using high-performance liquid chromatography (HPLC). Plasma samples were deproteinized; sildenafil was used as an internal standard. Chromatographic separation was achieved using a reversed-phase (C18) column. The mobile phase, 0.02 M ammonium acetate buffer:acetonitrile (48:52, v/v), was run at a flow rate of 1.0 mL/min at room temperature, and the column eluent was monitored using an ultraviolet detector at 280 nm. The retention times of JW-55 and sildenafil were approximately 5.9 and 7.7 min, respectively. The detection limit of JW-55 in rat plasma was 0.03 mg/mL. Pharmacokinetic parameters of JW-55 were evaluated after intravenous and oral administration of JW-55 (10 mg/kg) in rats. After oral administration, the F value was approximately 73.7%.

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발표분야: 의약화학
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An Efficient Synthesis of Imidazole[4,5-c][1,2]thiazine using a Solid-phase

김다현 이두현 이태호*

경북대학교 약학과

Solid-phase synthesis has become an powerful technique for the rapid generation of small, drug-like organic molecule libraries for pharmaceutical industry. Previously, we have studied about the construction of heterocyclic compounds via solid-phase synthetic strategy since they are often important structural components of bioactive molecules. So we have an interested in heterocyclic compounds containing imidazole moiety. Imidazole and thiazine moiety have various bioactivities, for instance the substituted imidazole derivatives are valuable in treatment of many systemic fungal infections. Imidazoles belong to the class of azole antifungals, which includes ketoconazole, miconazole, and clotrimazole. In This study we have led to the development of the first traceless solid-phase synthetic protocol that efficiently generated 1,3,5,6–tetrasubstituted–1H- imidazolo[4,5-c][1,2]thiazin-4 (3H)one-2,2-dioxide derivatives. Moreover, this strategy enables the construction of a large library and potentially applies the preparation of other drug-like imidazole-fused ring system.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MEDI.P-421**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of 4th generation EGFR Inhibitors overcoming EGFR C797S mutation for lung cancer treatment

전병욱 최현정[1] 신인지[2] 전문국[2] 채종학[3] 최길돈[4] 이광호[5,*]

서강대학교 화학과 [1]KAIST 화학과 [2]한국화학연구원 의약화학연구센터 [3]한국화학연구원 신물질연구본부/신약플랫폼기술팀 [4]한국화학연구원 의약바이오연구본부 [5]한국화학연구원 신물질본부/난치성

Erlotinib (Tarceva) & Gefitinib (Iressa) are the first class of drugs as epidermal growth factor receptor (EGFR) kinase inhibitors for non-small cell lung cancer (NSCLC) treatment. However, their clinical use is ultimately limited due to the mechanism-based toxicity and development of drug-resistance EGFR T790M mutation. Osimeritinib (Tagrisso), an irreversible inhibitor, has recently approved as for the next generation treatment option to overcome the short-comings of the first class drug use. Latest Osimeritinib clinical trial report reveals new acquired-resistant mechanism: EGFR C797S mutation showing limit of the irreversible inhibitors. In this presentation, new medicinal chemistry strategy is discussed to address the currently unmet-medical needs for EGFR-related NSCLC patients. Reversible pyrimidine-based inhibitors are explored to overcome EGFR L858R/T790M/C797S and EGFR ex19del/T790M/C797S triple mutants for effective clinical treatment for NSCLC patients.

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발표코드: **MEDI.P-422**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Construction of a Novel of 1H-benzo[d]imidazole-2-thiol Derivatives via nucleophilic cleavage reaction on Solid-Phase

<u>윤효정</u> 김예지 공영대*

동국대학교 화학과

In this experiment, we constructed N-alkyl-1H-benzo[d]imidazole-2-thiol derivatives on solid-phase synthesis. Substituted 1,2-phenylenediamines were used as starting material and protected with Boc group which then reacted 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. For further divercification, we conducted Suzuki coupling reaction at the C-X position. Finally, our desired product was successively obtained via nucleophilic cleavage reaction by benzyl thiol and potassium tert-butoxide in dimethylforamide (DMF) in high yields and good purities.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly Efficient Synthetic Method on Pyroacm ResinUsing the Boc SPPS Protocol for C-terminal Cysteine Peptide Synthesis

김강태 **JUVEKARVINAYAK** 공영대*

동국대학교 화학과

A one and two-step cleavage process of Pyroacm resin using trifluoromethanesulfonic acid and carboxymethylsulfenyl chloride was developed for solid phase peptide synthesis of C-terminal cysteine and cysteine ester peptides. The process uses cysteine side chain anchoring to the pyroacm resin and the Boc protocol for SPPS. TFMSA cleavage of protecting groups generates a peptide-linked resin, which can be subjected to peptide modification reactions.

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장소: 일산 KINTEX
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발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Construction of 1,3,4-Oxadiazole and 1,3,4-Thiadiazole Analogues via Desulfurative Cyclization of Thiosemicarbazide on Solid-phase synthesis

하지은 한시연 공영대*

동국대학교 화학과

In this work, we described synthesis of 1,3,4-oxadiazole and 1,3,4-thiadiazole derivatives on solid-phase synthesis. This solid-phase synthesis involves the preparation of 1,3,4-oxadiazole and 1,3,4-thiadiazole core skeleton resin through cyclization of thiosemicarbazide derived from a reaction between isothiocyanate resin and various hydrazides. To obtain 1,3,4-oxadiazole and 1,3,4-thiadiazole from thiosemicarbazide, we used EDC·HCl and p-TsCl, respectively. The resulting 1,3,4-oxadiazole and 1,3,4-thiadiazole resin was diversified by alkylation, acylation, suzuki coupling, reductive amination, and amide/urea formation and then followed by cleavage reaction under TFA in DCM to afford desired 1,3,4-oxadiazole and 1,3,4-thiadiazole analogues in good yields and high purities

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MEDI.P-425**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Solid-Phase Synthesis of 1,3,4-Thiadiazole Derivatives via DesulfurativeCyclization of Thiosemicarbazide Intermediate

양승주 **ABDILDINOVA AIZHAN** 정선화 공영대*

동국대학교 화학과

A 1,3,4-thiadiazole library was constructed by solid-phase organic synthesis. The key step of this solid-phase synthesis involves the preparation of polymer-bound 2-amido-5-amino-1,3,4- thiadiazole resin by the cyclization of thiosemicarbazide resin using p-TsCl as the desulfurative agent, followed by the functionalization of the resin by alkylation, acylation, alkylation/acylation, and Suzuki coupling reactions. Both the alkylation and acylation reactions chemoselectively occurred at the 2-amide position of 2-amido-5-amino-1,3,4-thiadiazole resin and the 5-amine position of 2-amido-5-amino-1,3,4-thiadiazole resin, respectively. Finally, these functionalized 1,3,4-thiadiazole resins were treated with trifluoroacetic acid in dichloromethane, generating myriad of 1,3,4-thiadiazole analogs in high yields and purities. The 1,3,4-thiadiazole derivatives show a different distribution of physicochemical and biological properties compared to our previously constructed 1,3,4-oxadiazole and 1,3,4-thiadiazole libraries in a range of orally available drug properties.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-426**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of 1-alkyl-N-alkyl/acyl-1H-benzo[d]imidazole-2-aminederivatives via desulfurative cyclization on solid-phase organic synthesis

유현정 권혜진 공영대*

동국대학교 화학과

In this study, we synthesized 1-alkyl-N-alkyl/acyl-1H-benzo[d]imidazole-2-amine derivatives. 2-Fluoronitro benzene was used as a starting material and reacted with various amines. With the N-alkyl-2-nitroanilines in hand, N1-alkylbenzene-1,2-diamines were obtained through a reduction reaction. Next, N1-alkylbenzene-1,2-diamines reacted with polymer supported isothiocyanate derived from 4-benzyloxy-2-methoxybenzylamine (BOMBA) resin through a reaction with carbondisulfide, trimethylamine p-TsCl in tetrahydrofuran to generate thiourea intermediate resin. The cyclization of thiourea intermediate resin was successfully conducted through desulfurative cyclization with 2-chloro-1,3-dimethylimidazolinium chloride (DMC) and N,N-diisopropylethylamine in dichloromethane (DCM). Next, various electrophiles such as alkyl halide, acid chlorides were introduced at 2-amine position. Finally, we obtained various 1-alkyl-N-alkyl/acyl-1H-benzo[d]imidazole-2-amine by cleavage of the corresponding resin under trifluoroacetic acid (TFA) in dichloromethane (DCM).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-427**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Dipyrrolopyrazine (DPP) Derivatives via Metal Free and Metal Catalyzed Regioselective Amination and Investigation of Their Optical and Thermal Properties

Puttavva meti 이은실[1] 공영대[*]

동국대학교 화학과 [1]동국대학교 의약화학연구실

Pyrazine is an important molecular scaffold employed in organic optoelectronic materials. Here we report efficient methods for the synthesis of dipyrrolopyrazine, and pyrrolothieno-pyrazine derivatives that involve regio-selective amination reactions of dihalo-pyrrolopyrazines. The developed protocol readily affords either 2-amino- or 3-amino-pyrrolopyrazines from the corresponding 2-bromo-3-chloro-5H-pyrrolo[2,3-b]pyrazines. When the amination reactions are carried under metal free under microwave irradiation, 3-amino-pyrrolopyrazines are obtained exclusively. In contrast, Buchwald cross coupling of the 2-bromo-3-chloro-5H-pyrrolo[2,3-b]pyrazines affords only 2-amino-pyrrolopyrazine. The pyrrolopyrazine scaffolds were converted to the respective 1,7- and 1,5-dihydrodipyrrolo[2,3-b]pyrazines derivatives using Sonogashira reactions. A comprehensive study of the optical properties, thermal properties, and molecular packing of the synthesized compounds was carried out. The results indicate that the 1,7-derivatives may be promising organic materials for optoelectronic applications.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MEDI.P-428**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparison of ISE and ICP-MS to Determine Iodine in Urine

조효정

녹십자의료재단 대사체연구팀

Iodine, an essential element for thyroid function, is necessary for normal growth, development, and functioning of the brain and body. Iodine-deficiency disorder (IDD) is a well documented global health problem, affecting more than a billion people worldwide. Consequences of IDD include goiter, cretinism, intellectual impairment, brain damage, mental retardation, stillbirth, spontaneous abortions, miscarriages, congenital deformities, and increased perinatal mortality. Urinary iodine values directly reflect dietary iodine intake, urinary iodine analysis is the recommended and most common method for biochemically assessing the iodine status of a population. This method achieves rapid and accurate quantification of iodine content in urine. We evaluated the analytical performance of inductively coupled plasma-mass spectrometry (ICP-MS) and Ion-selective electrodes (ISE) to determine urinary iodine concentration. And the 2 methods for iodine were compared for the 24hr urine samples(n=105).Material & Method• ICP-MS method 20 uL of the internal standard solution (Indium, 100ug/L) and 2 mL of dilution solution (0.05% triton X-100, 0.2% NH4OH, 2% 1-butanol, 0.05% ehtylendiaminetetraacetic acid diammonium salt hydrate in d.w) were added into 100 uL of urine then vortex mixed for 30 sec. And injected into the 7900x ICP-MS system(Agilent, USA). - Iodine (127) - Indium (IS) (115)• ISE method40 uL of the ISA solution and 1.8 mL d.w were added into 200 uL of urine then vortex mixed for 30 sec. And injected into the A214 ISE iodide electrode. (Thermo, USA).ConclusionThe difference % of two methods is within a ±20%. But ISE method is lower precision than ICP-MS and value have increased over time. It seems that iodine in urine is not entirely free iodide, and free iodine becomes increasingly with time. ISE electrode is influenced by pH, acids, matrix etc. So the application of ISE is often necessary quality control to check the accuracy.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-429**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Chemical Biology Approach for the Identification of Cell Protecting Molecules

김동희 이희수[1] 이재욱[2,*]

한국과학기술연구원 치매DTC연구단 [1]강릉원주대학교 치의학과 [2]한국과학기술연구원(KIST) 치매DTC융합연구단

Chemical biology approach is one of most powerful methods to discovery biologically active molecules. By conjugation of HTS (high throughput screen), this approach can leverage automation to search drug like compounds based on cell based or biochemical based assay. Discovering active compounds that affect biological functions will lead to identification of novel biologically functional components and establish the basis for therapeutic strategies. Beta cell dysfunction or death plays crucial roles in the progression of type 1 and type 2 diabetes. Current anti-diabetic drug cannot prevent the progression of beta cell dysfunction and death. In diabetes, major cause of beta cell dysfunction and death is related with endoplasmic reticulum (ER) stress. By using chemical biology approach, we identified quinazoline compounds as a novel class of β-cell protective agents against ER stress-induced dysfunction and death. Through extensive SAR optimization, 2,4-diaminoquinazoline markedly protects β-cells against ER stress-induced dysfunction and death with 80% maximum rescue activity. We are currently under further investigation for animal model studies to evaluate efficacy of the compound.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MEDI.P-430**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Highly Enhanced Photodynamic Activity of Purpurinimide Derivatives and Nanocarrier Effect

윤일* 심영기[1]

인제대학교 PDT 연구소 [1]인제대학교 나노융합공학부

Purpurinimide derivatives and its polyoxometalate as well as graphene oxide complexes as nanocarriers were synthesized, and their excellent photodynamic activity results were obtained based on excellent nanocarrier effect, resulting in significantly enhanced PDT activity. Cellular uptake images and cell viability results are shown.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MEDI.P-431**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

PreMetabo: Software for drug metabolism prediction

황성보 신성은[1] 서명원 신현길 노경태[*]

연세대학교 생명공학과 [1](사)분자설계연구소 화학생물정보연구팀

Drug metabolism in hepatocytes attracted many researchers' interests since metabolism reactions alter toxicity and efficacy of drug molecules. Researches on metabolism revealed the proteins playing major role in drug metabolism; cytochrome P450 enzymes (CYPs) for phase I reaction, UDP-glucuronosyltransferases (UGTs) and sulfotransferases (SULTs) for phase II reaction, and P-glycoprotein (P-gp) for transportation of drug molecule."PreMetabo" is user-friendly software to predict metabolism of drug molecules for helping users to make decision in early stage. It is named by combining the words 'prediction' and 'metabolism.' Metabolism predictions are useful to understand fate of drug molecules in hepatocytes. The software is composed of modules to predict site of metabolism by CYPs, and to classify substrate of CYP2D6, CYP3A4, UGT, SULT, and P-gp, or inhibitor of CYP2C9, CYP2C19, CYP2D6, and CYP3A4. PreMetabo is not only implemented as GUI version, but also as web version to make it accessible to everyone. (https://premetabo.bmdrc.kr/)

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발표코드: **MEDI.P-432**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Development of phase 1 and phase 2 drug metabolism prediction model

신성은 황성보[1] 서명원[1] 신현길[1] 노경태[1,*]

(사)분자설계연구소 화학생물정보연구팀 [1]연세대학교 생명공학과

Toxicity and efficacy of drug can be altered through metabolism reactions in hepatocyte; therefore, prediction on drug metabolism in early phase can give benefits in drug discovery process. In this work, phase I and phase II metabolism prediction models were introduced. Phase I reactions of drug metabolism are mainly driven by cytochrome P450 enzymes (CYPs), which modify functional groups on drug. For phase I metabolism, metabolized site in the molecule, called the site of metabolism (SOM) was predicted by binding energy with the molecule and the CYPs, and activation energy of SOM with heme group of CYPs. Majority of phase II reactions is conjugation reaction, adding certain molecules on the xenobiotics. For phase II metabolism, classification models were developed to predict whether the molecule is a substrate of UDP-glucuronosyltransferases (UGTs). Consensus approach was applied to predict phase II metabolism with support vector machine and logistic regression models.

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발표코드: **MEDI.P-433**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

The Simultaneous Analysis of Essential Trace Elements in Human Breast Milk by ICP-MS

조효정

녹십자의료재단 대사체연구팀

Recently, analytical methods have some light on the nutritional importance of essential elements in human breast milk. Trace elements analyses in human breast milk have been previously reported using various methologies. ICP-MS has become one of the most sensitive, accurate and reliable analytical techniques for determination of trace elements. Previous studies have reported involving microwave with acid digestion at various temperatures. But this methods are time-consuming and expensive, highly losses by volatilization, contamination, hazardous use of mineral acids.The main objectives this study were to determination trace elements(Zn, Cu, Mn) and stability in human breast milk.Material & Method• Study sampleA certified reference material for human breast milk is currently not available, and pooled human breast milk samples as well as standard reference materials for formula milk powder such as NIST 1549a to validate the methods.All samples were frozen at -20℃ until analysis. And samples were thawed at room temperature. • ICP-MS method 80 uL of the internal standard solution (Indium, 100ug/L) and 1.6 mL of dilution solution (2% HNO3 and 0.01% triton X-100 in d.w) were added into 160 uL of sample. It vortex mixed for 30 sec and centrifuge 13,200 rpm, 4℃. Injected into the 7900x ICP-MS system(Agilent, USA). - Manganese (55), Copper(63), Zinc(66) - Indium (Internal standard) (115)ConclusionThe method is precise with intra-day and inter-day repeatability values of

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-434**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis and Biological Evaluation of the Novel SHIP2 Inhibitors for the Treatment of Alzheimer's Disease

임지웅 배애님[1,*] 이재열[2] 이재욱[3] 김동회[4] 임상민[5]

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Inositol polyphosphate 5-phosphatase (SHIP2) is an important negative regulator of intracellular phosphatidylinositol phosphate, a key second messenger of various intracellular signaling pathways. Recent studies have suggested that inhibition of SHIP2 could produce a significant benefits in the treatment of Alzheimer's Disease (AD). It is characterized by amyloid-β (Aβ) plaques in the brain and neurofibrillary tangles of hyper-phosphorylated tau, a microtubule-binding protein. The FcgRIIb-SHIP2 signaling axis could provide the missing link between Aβ and tau pathologies. Notably, Aβ1-42 induces FcgRIIb phosphorylation to recruit SHIP2, followed by increased production of PIP2(3,4), disrupting the balance of phosphoinositide metabolism leading to tau hyperphosphorylation and memory impairment in neurons. Therefore, inhibition of SHIP2 can be an effective therapeutic strategy in AD. For developing SHIP2 inhibitors, we performed the phosphatase assay with malachite green using in house libraries. From high-throughput screening, we found hit compounds, and synthesized new derivatives based on the hit scaffolds. Among the synthesized compounds, DTC0217 was identified as a potent SHIP2 inhibitor. The optimization of novel SHIP2 inhibitors to further enhance potency and physicochemical properties is now in progress. We have presented the first example of a small molecule SHIP2 inhibitors for AD. This compound will help to elucidate physiological functions of SHIP2 and its involvement in AD.

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Development of Tau Aggregation Inhibitors for Treatment of Alzheimer's Disease

이하은 배애님[1,*] 임상민[2]

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Alzheimer's disease (AD) is one of the most common neurodegenerative diseases and becomes a severe problem in an aging society. Tau protein plays an important role in AD pathology. Tau is a microtubule-associated protein and, helps to stabilize neuronal microtubule. But hyperphosphorylation of tau leads to disengage it from the microtubule, which results in self-assembly of tau forming paired helical filaments (PHFs) and neurofibrillary tangles (NFTs). Finally, these PHFs and NFTs induce neuronal damage like AD. Although tauopathy has been extensively studied as a key hypothesis in AD there are no clinical drugs to give the noticeable improvement. Therefore, we study to find Tau-directed therapeutic drug candidates for the treatment of AD, especially, tau aggregation inhibitors. To discover new lead compounds that can inhibit tau aggregation, we performed a high-throughput screening based on Bi-FC assay with in-house and commercial compound libraries. Subsequently, we found hit compounds that are more potent and less toxic than the Methylene blue: a well-known in vitro tau aggregation inhibitor. Currently, a variety of derivatives were synthesized through a structure-activity relationship study to find compounds that are more potent and possess novel scaffolds than the hit compounds. We will continue to work to further optimize potency as well as physicochemical properties to develop clinical candidates.

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Novel urotensin-II antagonist

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Among many targets, urotensin-II receptor (UT) has attracted considerable recent attention as a therapeutic target for treatment of heart failure. Urotensin-II (U-II), a cysteine-linked cyclic peptide, is mainly expressed in a variety of tissues, including blood vessels, heart, liver, kidney, skeletal muscle and lung. It is known to be the most potent vasoconstrictor, displaying a 10 times greater potency than that of endothelin. The effects of this peptide are mediated through its interaction with a G protein-coupled receptor known as a GPR14 or the urotensin-II receptor. Activation of UT by binding with U-II results in several cardiovascular responses including vasoconstriction, vasodilation, cell proliferation and hypertrophy. These findings suggest that U-II and its receptor system are involved in the pathogenesis of cardiovascular disease. Furthermore, the results of previous studies demonstrate that the expression of UT is low or undetectable in normal myocardium, whereas elevated U-II plasma levels and increased levels of UT expression are associated with numerous cardiorenal and metabolic diseases, including hypertension, heart failure, atherosclerosis, diabetes and renal failure. Therefore, UT has emerged as one of the most promising therapeutic target for treatment of heart failure as well as a broad range of other cardiovascular maladies. As part of a continuing program aimed at the development of novel and potent UT antagonists, we recently identified and optimized a series of aminopiperidine derivatives. The details of synthesis, biological evaluation and structure-activity relationships(SAR) results will be discussed.

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Radiosynthesis of [^{68}Ga]Ga-PSMA-11 with customized synthetic module for routine clinical use

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[^{68}Ga]Ga-PSMA-11 ([^{68}Ga]Ga-PSMA-HBED-CC) has been widely employed as efficient PET imaging agent for early diagnosis of prostate cancer. For the routine supply of prostate-specific membrane antigen (PSMA) radiotracer in the clinics, we aimed to develop a reliable method to produce [^{68}Ga]Ga-PSMA-11 using in-house built radiolabeling platform. Herein, we report the automatic radiosynthesis of [^{68}Ga]Ga-PSMA-11 for routine clinical application. For the optimal ^{68}Ga chelation, the first eluate (1.5 mL, 0.6 M HCl) from SnO_2-based generator (iThembaLABS) was discarded. [^{68}Ga]Eluate (2.5 mL, 1332-1369 MBq) from generator was introduced directly to the vial containing HEPES powder (500 mg) and stirred (pH 3-3.5) while heating. When HEPES was completely dissolved at 95 ^{o}C, PSMA-11 precursor (10 μg) in H_2O (0.2 mL) was added for complete ^{68}Ga chelation at 95 ^{o}C for 10 min. Final product was purified using SPE cartridge (Strata X C18, Phenomenex) and washed with H_2O (10 mL) to remove residual HEPES. [^{68}Ga]Ga-PSMA-11 was isolated with EtOH (0.7 mL) and formulated with 0.9 % saline (9 mL). [^{68}Ga]Ga-PSMA-11 was produced in 95-98 % RCYs (925-962 MBq, n = 10) with radiochemical purity above 98%. Overall preparation time was *ca*. 30 min. The purity of [^{68}Ga]Ga-PSMA-11 was verified by iTLC (eluent: 50% MeOH/NH_4OAc, v/v). The residual HEPES content was determined by HPLC. This house-built automated module was proved to be efficient and economical protocol compared to commercially available alternatives. This work was supported by the National Research Foundation (NRF) of Korea, funded by the Ministry of Science (No. 2015R1D1A1A02061420).

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QSAR Modeling for hERG Inhibition by Learning Machine Methods

서용일 남기엽* 서영주 문자연 김민경 윤정혁[1]

(주)파로스아이비티 바이오인공지능연구소 [1](주)파로스아이비티 -

The hERG (the human Ether-à-go-go-Related Gene) is a one of ion channel protein to transport the potassium ions to selective. This gene contributes to the electrical activity of the heart such as QT interval. If the hERG ion channel does not play a role due to genetic or artificial factors, it will cause a long QT syndrome. Therefore, many drug candidates are dropped when they bind to hERG or interfere with the passage of potassium ions. There conduct an experiment in vitro like measuring half maximal inhibitory concentration (IC50) to prevent it. In recently, some compounds predict at risk for hERG inhibition using QSAR model before in vitro test. This study builds QSAR Models to predict hERG inhibitior qualitatively and quantitatively by using various machine learning methods such as MLR, LR, SVM, and ANN. We collect compounds through ChemBL for targeting with hERG and select training set by the experimental method, cell environment, and measurement method. Additionally, the compounds for quantitative prediction were selected so that the distribution of the experimental values was similar. To qualitative prediction, the experimental value of the compound is defined as Active and Inactive by criteria on 10-5 M, and the training set is selected to have as a ratio of 1: 1.

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Design and synthesis of novel triazolo[3,4-d]pyridazin-3-yl pyridine-2-amine derivatives as novel Bruton's tyrosine kinase inhibitors

김덕운 정현석 황종연[1] 김필호[1] 류도현 조성윤[2,*]

성균관대학교 화학과 [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 난치성질환치료제연구센터

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. BTK inhibitors are anticipitated to be important clinical options for treatin rheumatoid arthritis and lupus. 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 novel triazolo[3,4-d]pyridazin-3-yl pyridine-2-amine 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 enzyme and cell-based assay.

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Increase in apoptotic effect of temperature and pressure controlled microwave (TPC-MW) processed Ginseng

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Ginseng, which is widely used in functional foods and as an herbal medicine, has been reported to reduce the proliferation of prostate cancer cells by mechanisms that are not yet fully understood. This study was designed to investigate the changes in ginsenoside content in ginseng after treatment with a temperature and pressure controlled microwave (TPC-MW) process and to verify the anticancer effects thereof. After TPC-MW conversion of ginseng, the content of ginsenosides Rg1, Re, Rb1, Rc, Rb2, and Rd in the extracts decreased, whereas the content of ginsenosides 20(S)-Rg3, 20(R)-Rg3, Rk1, and Rg5 increased. Antiproliferation results for the human cancer cell lines treated with ginseng extracts indicate that PC-3 cells treated with MG showed the highest activity with an half maximal inhibitory concentration of 48 mg/mL. We also showed that MG suppresses the growth of human prostate cancer cell xenografts in athymic nude mice as an in vivo model. This growth suppression by MG is associated with the inductions of cell death and autophagy.Therefore, heat processing by TPC-MW is a useful method to enhance the anticancer effect of ginseng by increasing the content of ginsenosides Rg3, Rg5, and Rk1.

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발표코드: **MEDI.P-441**
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Synthesis of Cholinesterase Inhibitor using Lipoic-benzyl triazole Derivatives

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Alzheimer’s disease (AD) is the most common neurodegenerative disease among the cause of dementia which can appear in the elderly people aged 65 or old. The cause of Alzheimer's disease is not yet known exactly. Alzheimer's drugs based on the cholinergic theory currently marketed for the treatment of AD patient. However, they have serious side effects. We have been researching to find out new candidate compounds as cholinesterase inhibitors. In this study, a series of triazol compounds coupled by Click reaction between propagyl lipoic amide and benzyl azides were synthesized and their *in vitro* cholinesterase [acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE)] inhibitory activities were evaluated. Benzyl azides were selected to study the structure-activity relationship (SAR) depended on the Claig plot; plotting the sigma constants of the Hammett equation (б) versus hydrophobicity (π). The IC_{50} value of compound 29 (-б, -π) is 8.4±0.5μM and it is comparable to that of galantamine (IC_{50} = 9.4±2.5μM against BuChE).

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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장소: 일산 KINTEX
발표코드: **MEDI.P-442**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Anti-oxidative and anti-cholinesterase compounds from Galla Rhois

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In our continuing search for anti-oxidative, anti-cholinesterase and anti-tyrosinase compounds from oriental medicinal plants, Galla Rhois was examined. Here we report the progress on the purification, biological activities and structural determination of the two isolated compounds. From the 100% methanol extract of Galla Rhois, solvent partition fractions were prepared by using n-hexane(14-GRM-H), chloroform(14-GRM-C), butanol(14-GRM-B) and water(14-GRM-W). Among them 14-GRM-B showed strong anti-oxidative, BuChE* inhibitory and anti-tyrosinase activities. The 14-GRM-B of Galla Rhois showed 84% DPPH radical scavenging activity, 81% BuChE inhibitory activity and 62% tyrosinase inhibitory activity at 100 ppm. Using a series of ODS open column chromatographic purification steps, two compounds, 14-GRM-B-333 and 14-GRM-B-335 could be purified. At 100 ppm, they showed anti-oxidative activity as 93.9, 94.5%, anti-tyrosinase inhibitory activity as 70.9, 89.6%, and AChE** inhibitory activity as 50.3, 64.7%, respectively. The structures of 14-GRM-B-333 and 14-GRM-B-335 were determined by 1H and 13C NMR and MS analysis. The structures of 14-GRM-B-333 and 14-GRM-B-335 were turned out to be methyl gallate and PGG(pentagalloylglucose), respectively. * BuChE : Butyrylcholinesterase, ** AChE : Acetylcholinesterase

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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A two-photon probe for lysosomal pH. Detection of colon cancer in a human tissue by two-photon microscopy

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Lysosome is membrane-bound organelle containing hydrolases that degrade endocytosed macromolecules to obtain the energy or dispose the waste. For optimum enzyme activity, the lysosomal pH is maintained at 4.5-6.0 in the normal cells. In the cancer cells, however, the pH is decreased to 3.8-4.7. To understand the effects of lysosomal pH on physiology, there are a few reports on two-photon (TP) probes that can determine the lysosomal pH in a live tissue. However, there is no report on the TP probe that can detect colon cancer in a human tissue. Herein we report that BH3 can effectively detect cancer cells in a human colon tissue.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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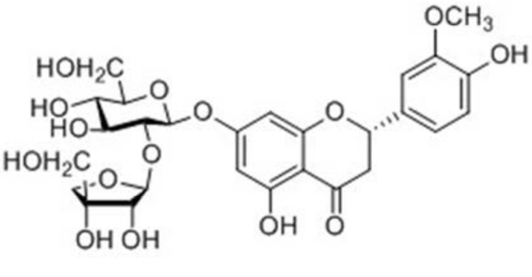
Identification of Viscumneoside III and Homoflavoyadorinin B isolated from korean mistletoe (Viscum album) and their anti-tyrosinase activity

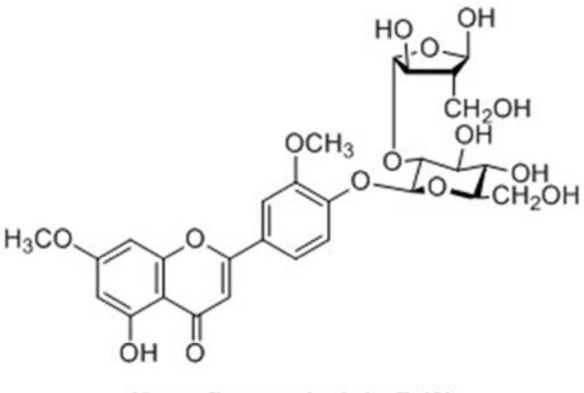
황운상 김재현 이구연*

강원대학교 생명건강공학과

Bioactive substances, viscumneoside III (1) and homoflavoyadorinin B (2), were isolated from EtOAc fraction of korean mistletoe. The identity of the compounds was verified by spectroscopic means including 1H NMR and mass spectrometry. All spectral data are consistent with reported values in the literature. The isolated compounds were performed to identify the effect on tyrosinase inhibition activity compared to ascorbic acid as a control. All compounds showed the higher whitening activity than these of control. These results revealed that the whitening acivity of Korean mistletoe can be utilized for the skin cosmetics. This work was supported by Korea Institute of Planning and Evaluation for Technology in Food, Agriculture, Forestry and Fisheries(IPET) through Export Promotion Technology Development Program, funded by Ministry of Agriculture, Food and Rural Affairs(MAFRA)(313011-03).



Viscumneoside III (1)



Homoflavoyadorinin B (2)

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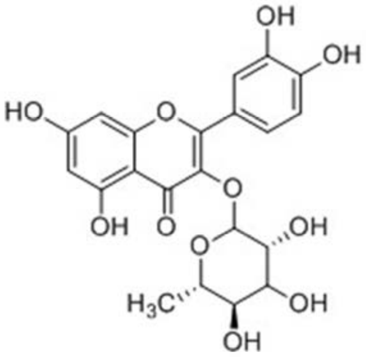
Discovery of rhamnoside derivatives as Tyrosinase Inhibitors from Loranthus tanakae

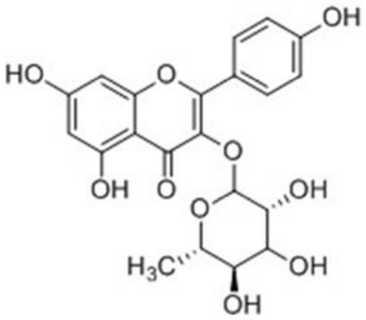
황운상 김재현 이구연*

강원대학교 생명건강공학과

Bioactive substances, quercetin 3-rhamnoside(1), kaempferol 3-rhamnoside (2), rhamnetin 3-rhamnoside(3), and rhamnocitrin 3-rhamnoside(4), were isolated from EtOAc fraction of Loranthus tanakae. The identity of the compounds was verified by spectroscopic means including 1H NMR and mass spectrometry. All spectral data are consistent with reported values in the literature. The isolated compounds were performed to identify the effect on tyrosinase inhibition activity compared to ascorbic acid as a control. Of the compounds, rhamnocitrin 3-rhamnoside(4) showed the higher whitening activity than these of control. These results revealed that the whitening acivity of Loranthus tanakae can be exploited for the skin cosmetics. This work was supported by Korea Institute of Planning and Evaluation for Technology in Food, Agriculture, Forestry and Fisheries(IPET) through Export Promotion Technology Development Program, funded by Ministry of Agriculture, Food and Rural Affairs(MAFRA)(313011-03).



Quercetin 3-rhamnoside (1)



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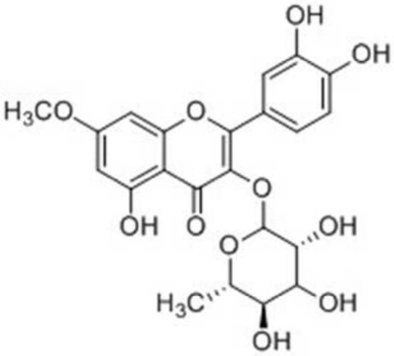
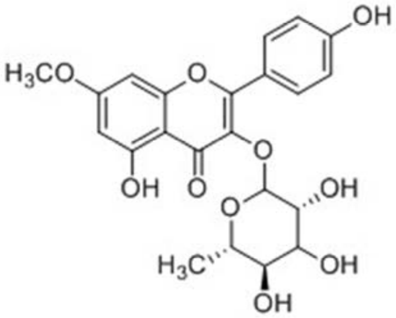


Rhamnetin 3-rhamnoside (3)



Rhamnocitrin 3-rhamnoside (4)

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장소: 일산 KINTEX
발표코드: **MEDI.P-446**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Discovery of small molecule inhibitors of Bromodomain Protein controlling c-Myc for treatment of cancers

유민진 조석준[1] 정관영[2,*]

과학기술연합대학원대학교(UST) 한국화학연구원/의약화학 [1]충북대학교 약학부 [2]한국화학연구원 의약화학연구센터

c-Myc is a regulator gene that codes for a transcription factor and overexpress in cancer cell. Indirect way of downregulation of c-Myc is the bromodomain inhibition. Bromodomain is a protein domain that recognizes acetylated lysine residues and control the c-Myc protein. We discovered 1*H*-indazole-4,7-dione scaffold using high throughput screening and synthesized a series of 1*H*-indazole-4,7-dione derivatives as a small molecule inhibitor of bromodomain protein. Among these synthesized small molecule inhibitors, 4*H*-1,2,4-triazolyl derivative represents the most potent inhibition effect toward c-Myc protein (IC_{50}= 0.24 μM). The result suggest that 1*H*-indazole-4,7-dione scaffold would be potent bromodomain inhibitor.

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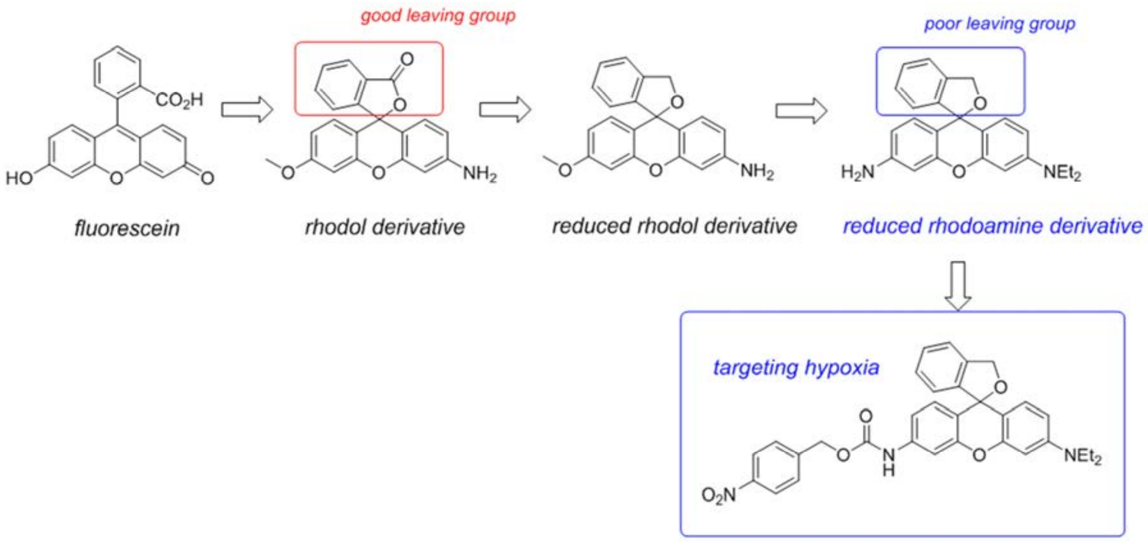
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Construction of New Reduced Rhodol and Rhodamine Fluorescent Probes with Chemical Stability and Their Application to Detection of Hypoxia

장동조* 강쥴리 MORE KUNAL <u>임태환</u>

순천대학교 약학과

With the recent advances of sensitive detection technology such as positron-emission tomography (PET) and fluorescent spectroscopy, there has been the demand for diverse imaging probes including fluorescent probes. Xanthene fluorophores including fluorescein, rhodamine and their hybrid structure, rhodol, are among the most commonly used fluorescent probes, and many activity-based fluorescent probes have been discovered with their asymmetric derivatives in many areas including biology and medicines. Of these fluorescent probes with xanthene structure, rhodol derivatives have been of great interest as activity-based fluorescent probes that can detect various phenonmena in live cells as well as metal ions because rhodol probes are fluorescent with a high quantum yield in aqueous solution within broad ranges of pH and are also known to be photo-stable as compared to other fluorescent probes such as fluorescein. However, as with fluorescein and rhodamine probes, rhodol probes also have a synthetic disadvantage that it’s difficult to modify and introduce diverse substituents at the terminal of xanthene ring due to low chemical stability to acids and bases. A few reduced fluorescein and rhodol fluorophores have been developed by several groups but the reduced rhodamine fluorescent probe has not been discovered. Herein, we describe a new reduced rhodamine fluorescent probes with chemical stability and its application to a new activity-based fluorescent probe to detect hypoxia.


good leaving group
poor leaving group
CO_2H
HO
O
NH_2
H_2N
NEt_2
fluorescein
rhodol derivative
reduced rhodol derivative
reduced rhodoamine derivative
targeting hypoxia
O_2N
N
H

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Development of Novel Anti-Hepatitis C Virus Agent Targeting NS5A

정유진 LIHUA[1] 강순방[1] 이정태 금교창[2,*]

한림대학교 화학과 [1]한국과학기술연구원(KIST) 뇌의약연구단 [2]한국과학기술연구원(KIST) 케모인포메틱스연구센터

Hepatitis C virus (HCV) is a leading cause of acute and chronic liver disease. About 180 million people are infected with HCV, which can lead to liver cirrhosis, hepatocellular carcinoma and consequently death. In addition to NS5B and NS3/4A protease inhibitor, NS5A was proved to be a promising target for the treatment of HCV. Several NS5A inhibitors such as BMS-790052 were launched recently and some were under clinical trials. We prepared a series of NS5A inhibitors possessing new scaffold and evaluated their activities against HCV cell lines. Among them, several compounds showed potent anti-HCV activity. Herein, we present anti-HCV activity of the hit compounds against various HCV genotypes and resistant strains mutated at L31V, Y93H of NS5A.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-449**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

국내 자생하는 참군소에 함유된 단일 화합물의분리 및 구조 규명 연구

김규선 최선준 김영석[1] 황병수[2] 전상일 함정엽[3,*]

강릉원주대학교 화학과 [1]한국과학기술연구원(KIST) 천연성분응용연구센터 [2]국립낙동강생물자원관 산업소재화연구부 [3]한국과학기술연구원(KIST) 천연물연구소

참군소(Aplysia kurodai)는 우리나라와 일본, 중국 연안에 서식하는 연체동물로 다양한 해조류와 저서성 규조류를 섭식하는 잡식성으로 알려져 있다. 군소에 함유된 성분과 활성에 대한 연구로 일본에서는 aplysin, aplysianin A, aplyronine A, B, C 의 분리 및 동정과 항암 활성이 있음을 보고한 바 있다. 국내 연구 사례로는 식용 가능한 군소육의 단백질 및 아미노산 조성에 관한 연구와 군소알의 열수 추출물의 항암 활성에 대하여 보고된 바 있으며, 내장 추출물로부터 항산화 및 항균효과를 보고한 연구들은 있으나 상대적으로 군소 자체의 화학적 성분과 활성에 관한 연구는 많이 되어 있지 않다. 본 연구자는 국내 연안에 자생하는 참군소를 메탄올로 추출하여 HPLC, MPLC, UPLC-MS 를 이용한 성분 분석 및 분리를 통해 단일 화합물들을 확보하였으며, FT-NMR 분석으로 각 성분들의 1D, 2D NMR 스펙트럼을 얻어 이들의 화학적 구조를 확인하여 dihydrorhodophytin, laureatin, debromolaurinterol, 4-hydroxydictylolactone 및 laurencin 임을 증명할 수 있었다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MEDI.P-450**

발표분야: 의약화학

발표종류: 포스터, 발표일시: 목 11:00~12:30

Synthesis of Chalcone Analogues That Protect Against Cisplatin-induced Cytotoxicity in LLC-PK1 Kidney Cells

김동희 이희수[1] 이재욱[2,*]

한국과학기술연구원 치매DTC연구단 [1]강릉원주대학교 치의학과 [2]한국과학기술연구원(KIST) 치매DTC융합연구단

Chalcones belong to one of largest class of plant metabolites and are known as precursors of flavonoids and isoflavonoids serving in plant defense mechanism to prevent damage from microorganism, insect, and animal. Therefore, chalcones and their derivatives have been reported to show a various biological activities such as anticancer, antiinflammatory, antiplasmodial, immunosuppressive and antioxidant properties. Acute renal failure (ARF) induced by either ischemia reperfusion or nephrotoxic drug was ameliorated by the treatment of chalcone analogues. Therefore, we synthesized Fifteen chalcone analogues to evaluate renoprotective effects using cisplatin-treated cultured kidney cells (LLC-PK1). In particular, chalcone derivatives 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.

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장소: 일산 KINTEX
발표코드: **MEDI.P-451**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel EGFR kinase inhibitors against EGFR T790M mutation

류희윤 손정범 강동욱[1,*] 최환근[*]

대구경북첨단의료산업진흥재단 신약개발지원센터 [1]대구가톨릭대학교 제약산업공학과

Kinase inhibitors have been playing an important role in the treatment of cancer and other diseases. However numerous reports indicate that patients end up gaining drug resistance towards those widely used drug. Among those, approximately 60% of the first generation of EGFR TKI (Epidermal Growth Factor Receptor Tyrosine Kinase inhibitor) for the treatment of non-small cell lung carcinoma (NSCLC), such as Gefitinib and Erlotinib, lost significant efficacy due to the emergence of EGFR-T790M gatekeeper mutation. In oreder to overcome this disturbing phenomenon, one needs to come up with a new agent that could not only be potent against EGFR-T790M, but also be selective over wild type EGFR. With respect to this, most of the second and third generation EGFR TKI (Afatinib, AZD-9291, CO1686, HM61713 and etc) possess acryl amide moiety that could form an irreversible bond with the cystein residue(C797). In the study, we report new type of irreversible inhibitors could form a covalent bond with EGFR-C797. Particularly, compound 2 has EGFR-T790M enzyme activity in EGFR-T790M (IC50: 5nM).

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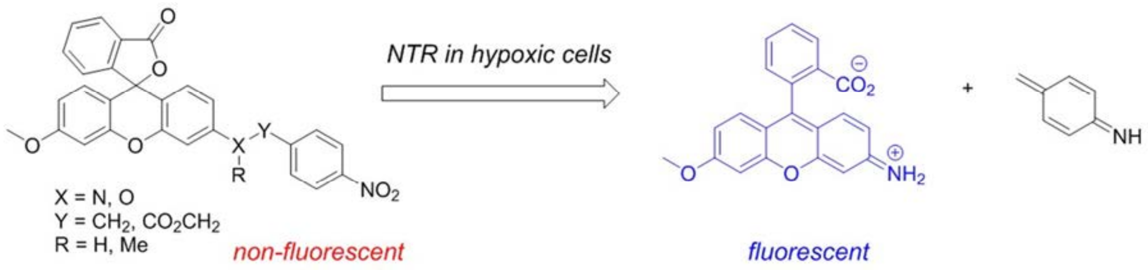
장소: 일산 KINTEX
발표코드: **MEDI.P-452**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

New Rhodol-Based Fluorescent Probes Targeting Hypoxia and Evaluation of Their Photochemical Properties

장동조* 강즐리 임태환 <u>MORE KUNAL</u>

순천대학교 약학과

Hypoxia is one of major phenomena in metastatic and solid tumors and affects the therapy of tumor by preventing the proper metabolism of anticancer agents. Many clinical research has revealed that tumor hypoxia shows a correlation with a resistance to chemotherapy and radiotherapy. Also, it has been known that the neovascularization in growing tumors leads to the angiogenesis of diverse tumors which results in poor prognosis and resistance to chemotherapy and radiotherapy. Since the discovery of 2-nitroimidazoles as a functional group capable of making irreversible adducts with nucleophilic macromolecules in hypoxic cells, hypoxia-activated drugs have been of great interest and investigated to develop diagnostic and therapeutic agents targeting hypoxia in various types of cancers. With the recent advance in optical sensing devices, fluorescence technology has been of extensive interest in many areas including biology and medicines as well as materials due to its high sensitivity. Of various fluorophores, only a few fluorescent probes have been discovered as activity-based fluorescent probes that can detect nitroreductase (NTR) in hypoxic cells. Our group have tried to discover new rhodol-based fluorescent probes with various functional groups detecting hypoxia because rhodol fluorophore shows high fluorescence in aqueous solution in broad ranges of pH and are also known to be resistance to photobleaching. Herein, we describe new rhodol-based fluorescent probes capable of detecting and imaging NTR, highly expressed protein in hypoxic cells, and evaluation of their photochemical properties as activity-based fluorescent probes targeting hypoxia.


NTR in hypoxic cells
X = N, O
Y = CH2, CO2CH2
R = H, Me
non-fluorescent
fluorescent
O
X
Y
R
NO2
CO2
NH2
NH
+

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장소: 일산 KINTEX
발표코드: **MEDI.P-453**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Identification of a novel 5-amino-3-(5-cyclopropylisoxazol-3-yl)-1-isopropyl-1H-pyrazole-4-carboxamide as a specific RET kinase inhibitor

신인재 심태보[1,*]

고려대학교 NBIT [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

Activating mutations of REarrange during Transfection (RET) kinase frequently occur in human thyroid and lung cancers. An enormous effort has been devoted to discover potent and selective inhibitors of RET. Selective and potent inhibitors against constitutively active RET mutants are rare to date as identification of selective RET inhibitors is challenging. In a recent effort we identified a novel and specific RET inhibitor of 5-aminopyrazole-4-carboxamide scaffold, which was designed to enhance the metabolic stability of the pyrazolopyrimidine scaffold. In the SAR study described in the current report, we identified the 5-aminopyrazole-4-carboxamide analog 15l, which displays high metabolic stability. Compound 15l is potent against gatekeeper mutant (IC50 = 252 nM) of RET as well as against wild-type RET (IC50 = 44 nM). This substance effectively suppresses growth of Ba/F3 cells transformed with wild-type RET and its gatekeeper mutant (V804M), and thyroid-cancer derived TT cells while it does not affect parental Ba/F3 cells and Nthy ori-3-1, normal thyroid cells. Also, the results of a global kinase profiling assay on a panel of 369 kinases, show that 15l exclusively inhibits RET. Based on its exceptional kinase selectivity, great potency and metabolic stability, 15l represents a promising lead for the discovery of RET directed therapeutic agent and should be a key tool in studies aimed at understanding RET biology.

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Identification of the First Selective Activin Receptor-Like Kinase 1 Inhibitor, a Reversible Version of L-783277

조한나 심태보[1,*]

고려대학교 KU-KIST [1]한국과학기술연구원(KIST) 화학키노믹스연구센터

We synthesized 1 (San78-130), a reversible version of L-783277, as a selective and potent ALK1 inhibitor. Our study showed that 1 possesses great kinase selectivity against a panel of 342 kinases and more potent activity against ALK1 than L-783277. Among the six ALK isotypes (ALK1−6), ALK1 is most significantly inhibited by compound 1. Compound 1 suppresses the BMP9-induced Smad1/5 pathway by mainly inhibiting ALK1 in C2C12 cells. Our molecular dynamics simulations suggest that H-bonding interaction between the C-4′ hydroxyl group of 1 and Arg334 of ALK1substantially contributes to the ALK1 inhibition. To the best of our knowledge, 1 is the first selective ALK1 inhibitor. Furthermore, compound 1 promoted angiogenesis in both endothelial tube formation and microfluidic chip based 3D angiogenesis assays, suggesting that 1 could be a lead compound for therapeutic angiogenesis agents. Our study may provide an insight into designing selective and potent inhibitors against ALK1.

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Synthesis of A2B corroles for the application of photodynamic therapy

선경표 윤새미 석지수 백지현[1] 이은규[1] 하용황[1,*]

중원대학교 의약화학과 [1]중원대학교 의약바이오학과

Many researches are interested in developing tumor-specific destruction method. As an alternative therapeutic skill, photodynamic therapy (PDT) attracts great interest due to its high selectivity to tumor cells. PDT is based on the photosensitizers which can generate singlet oxygen by energy transfer from triplet excited state sensitizers to molecular oxygens in ground state. Herein, we designed two types of A2B corroles and aluminum (III) 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.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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발표분야: 의약화학
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Recent biologically-oriented applications of corroles

윤새미 선경표 하용황[1,*]

중원대학교 의약화학과 [1]중원대학교 의약바이오학과

Various corrole compounds, which have very similar core structure with porphyrin, have been attracted many interests with respect to synthetic strategies and biological applications. Although photophysical properties of corroles are similar porphyrin molecules, biological characteristics exhibit more improved applicability for molecular imaging, detection and degradation of tumors, DNA sensors, catalytic degradation of reactive nitrogen species (RNS), and generation of singlet oxygen as photosensitizers. Herein, we reviewed photophysical properties, and examples of biological applications of corroles and discussed the structural characteristics of each application. We expected this review can be a basic study for corrole applications in biological and therapeutic studies.

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발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Targeted degradation of anaplastic lymphoma kinase (ALK): Design and synthesis of target degraducers (TDs)

이동호 장예린[1] 소민섭[2] 이덕형 하재두[3] 황종연[1,*]

서강대학교 화학과 [1]한국화학연구원 의약화학연구센터 [2]충남대학교 화학과 [3]한국화학연구원 난치성질환치료제연구센터

Recently, a new and powerful technology called "proteomosis targeting chimeras" (PROTAC) has been actively applied in the field of drug development. Treatment of PROTAC molecule, which contains a ligand for the targeted protein, a ligand for E3 ubiquitin ligase binding, and a linker for connection of two ligands, successfully induced targeted protein degradation, thereby inhibiting cancer growth in in vivo animal model study. Anaplastic lymphoma kinase (ALK) gene fused to various partner genes are observed in 3–7% of non-small cell lung cancer (NSCLC) in humans. The constitutively activated ALK fusions play an essential role in cancer growth and survival. In this study we aimed to discover novel ALK target degraders (TDs) by applying PROTAC technology. LDK-378 (ceritinib) as an ALK ligand and VHL or CRBN as an E3 ubiquitin ligase were used. Hydroxyproline analogs (HP-7) and pomalidomide were used for VHL and CRBN E3 ligase ligands, respectively. All TDs synthesized in this study were evaluated in enzymatic- and cell-based assays. ALK degradation by TDs were confirmed by western blotting in SU-DHL-1 cell lines. In vivo antitumor activities were evaluated in xenograft mouse model with H3122 cell lines.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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Discovery of novel 2,4-diaminopyrimidines bearing tetrahydronaphthalenyl moiety as ALK inhibitor

이동호 장예린[1] 이덕형 윤창수[1] 하재두[2] 황종연[1,*]

서강대학교 화학과 [1]한국화학연구원 의약화학연구센터 [2]한국화학연구원 난치성질환치료제연구센터

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.

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A Novel Class of Highly Potent Small Molecule Inhibitors of Rhinovirus Replication

김진우 정영식[1,*]

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Human rhinovirus (hRV) is a main causative agent of upper respiratory illness, namely common colds. The hRV infection also has been known to exacerbate asthma, acute otitis media and chronic obstructive pulmonary diseases (COPD), accompanying airway obstruction and hyperresponsiveness. The development of anti-hRV drugs has been hampered by the extreme diversity in hRV serotypes. Although several compounds have been shown anti-hRV activity, none of them have been approved yet.In this study, we disclose a novel series of 6-{[2-(methylcarbamoyl)pyridin-4-yl]oxy}benzo[*b*]thiophene-2-carboxylic ester derivatives against viral replication of hRV-A and hRV-B species. We found that compound KR-25763 have 2-digit nanomolar reactivity against both hRV species (EC_{50} = 0.053, 0.08 and 0.016 μM for hRV-B14, hRV-A21 and hRVA71, respectively). Time-of-addition study revealed that KR-25763 act as the early stage of the replication, namely the viral entry. Mutation study showed a single point mutation on Leu25 of viral capsid protein 3 (VP3) and computational study suggested the key interaction between KR-25763 and VP3 N-terminal chain. Cross resistance experiments displayed only partial cross resistance with pleconaril and vapendavir, previously reported potent capsid binding inhibitors. In addition, anti-poliovirus 3 (PV3) reactivity of KR-25763 implies its potential for the braod-spectrum reactivity against hRVs and other enterovirus species.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MEDI.P-460**
발표분야: 의약화학
발표종류: 포스터, 발표일시: 목 11:00~12:30

Novel Enterovirus Inhibitory Activity of 4-aryl-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 C_8-*tert*-butyl Group

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A series of 4-aryl-6,7,8,9-tetrahydrobenzo[4,5]thieno[3,2-*e*]triazolo[4,3-*a*]pyrimidin-5(4*H*)-one analogs (**A**), were prepared and tested for their inhibitory activity against representative enteroviruses. The activities were tested against Coxsackie Virus B1 (Cox B1), Coxsackie Virus B3 (Cox B3), Poliovirus 3 (PV3), Human Rhinovirus 14 (HRV14), Human Rhinovirus 21 (HRV21) and Human Rhinovirus 71 (HRV71). The C_8-*tert*-butyl group in these derivatives was found to be crucial for the activity of these compounds against these enteroviruses. Compound **5** as a racemic mixture showed single digit micro molar activity (1.6 - 8.85 micromoles) in the whole spectrum of viruses screened. Substitution on phenyl ring at N_4 position were tolerated, especially at ortho and para positions, among which compound **22** (*p*-methyl) and **29** (*p*-methoxy) being less cytotoxic, showed better selectivity indices against HRV14, HRV21 and HRV71 (selective index value range 4.6 - 12.2) compared to compound **5**. In general phenyl substitutions were more tolerated in PV3 and HRV’s compared to Coxsackie strains & showed improved cytotoxicity in rhinoviruses. Metabolic stability of the compounds evaluated experimentally which shows them to be promising for further development. The chiral separation of compound **5** resulted compound with much better activity profile than the racemic form **5**. The present study resulted in discovery of thienotriazolopyrimidinones as a novel skeleton as replication inhibitor of enterovirus.

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Benzo[d]oxazole derivatives as selective MAO-B inhibitors for treatment of Parkinson’s disease

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Parkinson’s disease is the second most common neurodegenerative disease in developed countries after Alzheimer's disease. Monoamine oxidase B as a mitochondrial bound enzyme is involved in catabolic oxidative deamination of dopamine. As the increased levels of MAO-B result in death of dopaminergic neurons in substantia nigra, MAO-B is considered as potential target for treating Parkinson’s disease. As a part of our continuous search for selective MAO-B inhibitors, a series of benzo[d]oxazoles are synthesized and structure-activity relationship (SAR) study was carried out. Among the synthesized benzo[d]oxazole compounds, compounds 8f and 8e are the most active compounds with IC50 values of 58.9 nM and 68.5 nM, respectively, which showed selectivity over MAO-A. We also performed the molecular docking study for the investigation of the binding mode of novel MAO-B inhibitors.

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[발표취소] Antitumor efficacy of docetaxel-loaded multi-layered nanoparticles

안주영 육순홍[1,*]

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장소: 일산 KINTEX

발표코드: **MEDI.P-463**

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[발표취소] 난용성 미백소재의 가용화를 통한 고효능 미백화장품 개발

이용우

충남대학교 신약개발학과

발 표 취 소

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Insights into the Interaction Mechanism of NAM and mGluR2: A Computational Modeling Approach

Gadhe Changdev Gorakshnath 배애님[1,*]

한국과학기술연구원(KIST) 치매DTC융합연구단 [1]한국과학기술연구원(KIST) 생체과학연구본부

Allosteric modulation of G protein-coupled receptors (GPCRs) represents a novel strategy for the development of subtype-specific therapeutics for the central nervous system target receptors. The metabotropic glutamate receptor 2 (mGluR2) is a class C GPCRs that plays an important role in neuro-modulatory brain functions. mGluR2 is an attractive drug target for the therapeutic intervention of neurodegenerative disorders including anxiety, depression, Fragile X Syndrome, Parkinson’s disease and schizophrenia. Unavailability of mGluR2 X-ray structure and implications in various neurodegenerative disease prompted us to initiate the computational modeling study. Therefore, we perform homology modeling to develop 3D-model of mGluR2. Computational docking studies of negative allosteric modulators (NAM) was executed in the predefined binding site. Ligand-protein complexes were embedded in hydrated palmitoylloleoylphosphatidylcholine (POPC) lipid bilayers, and these systems were simulated via molecular dynamics (MD) simulations to get robust, relaxed and better binding modes. Analyses of binding modes were performed, and pharmacophore models were developed and validated. Pharmacophore models were served to screen chemical libraries to get novel hits. ADMET filters were used to reduce the data size and compounds were purchased for biological testing. In future, lead optimization to be performed to get novel mGluR2 allosteric modulators for its therapeutic benefits in neurodegenerative disorder.

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[발표취소] Multivesicular Liposome Technology for the SustainedRelease of Bupivacaine

김경도* 허수진 강석희[1] 양태경[2]

충남대학교 약학과 [1]과학기술연합대학원대학교(UST) 한국화학연구원/의약화학및약리생물학 [2]충남대학교 응용화학공학과

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발표종류: 포스터, 발표일시: 목 11:00~12:30

[발표취소] Clustered Gold Coated Liposome for NIR-Triggered Photothermal Therapy

허수진* 김경도 양태경[1] 강석희[2]

충남대학교 약학과 [1]충남대학교 응용화학공학과 [2]과학기술연합대학원대학교(UST) 한국화학연구원/의약화학및약리생물학

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Dendrimer Based Nanocarriers for High Effective Delivery of Drugs in Photodynamic Therapy

<u>LIU YANG</u> 윤일[1,*]

인제대학교 school of nanoscienc [1]인제대학교 PDT 연구소

A dendritic polymer-photosensitizer complex was developed for noninvasive near-infrared fluorescence imaging and cancer therapy. In our group, we prepared unprecedented polymer-photosensitizer complex contains a lot of photosensitizers to generate high amount of ROS after light irradiation, resulting in enhanced PDT activity. Our result showed that (a)The new photosensitizer, purpurin-18-N-methoxyl, which has a long wavelength absorption (λmax 708 nm), that can allow deeper penetration of light to tumor tissue.(b) When we combine the dendrimer and PS .The ability to deliver more than one class of photosensitizer could be advantageous clinically, as the larger spectral region covered could lead to more efficient absorption of light; and (c) Based on the enhanced permeability and retention (EPR) effect of nanoparticles, it is expected that the polymer-photosensitizer complex can be accumulated in the extracellular space of tumors (it is not necessary to give a cellular internalization), which is very useful to kill cancer cells especially in vivo.(d) As a future work, 4th and 5th generations of dendrimer can make very powerful delivery systems with a large amount of photosensitizers for excellent PDT activity with good water solubility.

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pH-dependent hydrogen sulfide donors and their activity against myocardial ischemia-reperfusion injury

박정민

강릉원주대학교 화학신소재

Hydrogen sulfide (H_2S) has recently been identified as a physiologically important endogenous cell signaling molecule with potential therapeutic options for a diverse array of challenging diseases. In this presentation, we will report the design and synthesis of pH-dependent hydrogen sulfide releasing agents based on the phosphonamidothioate template and their potent cardioprotective effects in murine model of myocardial ischemia-reperfusion injury.

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발표코드: **MAT.P-328**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Cube-in-cube nanoparticles for super-radiant photoluminescence

박정은* 남좌민*

서울대학교 화학부

Photostability of photoluminescence (PL) from metal nanostructures such as non-photoblinking and non-photobleaching is beneficial to exploit them as reliable optical probes. The localized surface plasmon of plasmonic nanostructures strongly interact and concentrate light in the nanoscale allowing high absorption cross-section, which can compensate relatively low quantum yield (QY). However, recent studies on PL from plasmonic nanostructures have mostly been limited to lithographically fabricated structures or simple nanoparticles such as nanospheres or nanorods. Here we designed and synthesized interior nanogap-engineered cube-in-cube (CiC) nanoparticles (NPs) in a high yield via a galvanic void formation process.1 The CiC shows significantly enhanced PL and the PL intensity and QY of CiC NPs are 31 times and 16 times higher than those of Au nanocubes, respectively, which have the highest PL intensity and QY reported for metallic nanostructures. We attribute the intense PL to super-radiant character of plasmon mode arisen from plasmonic coupling between the core and the shell. Finally, we check the long-term photostability of the PL signal under continuous illumination for 1 h.

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Low-Voltage Organic Light-Emitting Field-Effect Transistors

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고려대학교 화학과 [1]고려대학교 일반대학원/화학과

In this study, organic light-emitting field effect transistors (OLEFETs) operating at low voltages of $|V_{op}| <$ 10 V were first produced and characterized. n-Dodecylphosphonic acid (PA-C12)-self-assembled monolayer (SAM)-passivated HfO_x dielectrics prepared using sol-gel chemistry were employed to decrease device-operating voltages. Pentacene and N,N′-ditridecylperylene-3,4,9,10-tetracarboxylic diimide acted as p-and n-type materials, and 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran doped into tris(8-hydroxyquinoline) aluminum layer was used as a light-emitting layer to improve the luminescence efficiency. Based upon the growth of well-packed crystalline organic active layers with ambipolar transports, and the high capacitance and low leakage current of the PA-C12-SAM-treated HfO_x dielectrics, the OLEFETs present good device performance with light emission at $|V| < 10$ V in air. The transistor characteristics and operating light-emission mechanisms were discussed based on EL photos acquired using a charge-coupled device camera.

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Structurally Controlled Electrum Nanostructures for Catalystic and SERS Applications

오주환 이재승*

고려대학교 신소재공학부

Bimetallic gold/silver nanostructures, or ‘electrum’ nanostructures have attracted particular attention because they not only retain the characteristics of both pure gold (Au) and silver (Ag) nanostructures but also exhibit enhanced chemical and physical properties owing to synergic combination of both characteristics resulting from monometallic nanostructures. In order to obtain desired chemical and physical properties, controlling the morphologies of bimetallic Au/Ag nanostructures has been of significant interest owing to their structure-dependent chemical and physical properties. To date, the synthesis of various bimetallic nanostructures including wire, rod, plate, frame, hollow, and core-shell structures have been demonstrated. These nanostructures, however, are typically limited to simple structures which were already widely investigated with monometallic nanostructures. Bimetallic Au/Ag nanostructures with high complexity are highly expected to extend the understanding for controlling the morphologies of bimetallic nanostructures. In this work, we demonstrate in-plate and on-plate structural control of Au/Ag bimetallic nanoplates (Au/Ag BNPLs). The Au/Ag BNPLs exhibit high chemical stability, and are utilized as redox catalysts for various catalytic reactions. Significantly, the Au/Ag BNPLs exhibit reversible assembly properties through surface modification, demonstrating the potential for diagnostic applications. Finally, the surface-enhanced Raman scattering (SERS) properties of the Au/Ag BNPLs are investigated as single nanoparticle SERS probes. electron microscopy, UV-vis spectroscopy, selected area electron diffraction, and energy dispersive X-ray spectroscopy are employed to analyze the structure and composition of the Au/Ag BNPLs at the atomic level.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Chemical buffer layer-armed high performance nanocatalysts for enhanced catalytic activity and stability

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Abstract Day by day global air and water resources have been seriously polluted owing to industrial progress. Since nanocatalysts have been considered one of powerful candidates for solving such a problem, purification of organic pollutants using catalysts has become an important issue in catalytic research and practical applications. 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 and Au catalysts.

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발표코드: **MAT.P-332**

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Amphiprotic all-in-one device for oil/water separation and pollutant purification

한나라 최원산*

한밭대학교 화학생명공학과

Abstract Global water resources have been continuously polluted due to industrial progress. Increasingly frequent oil spill accidents as well as industrial wastewater that contains oil have further led to the severe pollution of various water resources. Therefore, oil/water separation has recently become an important issue in scientific research and practical applications. We report a self-floating all-in-one device that simultaneously coexists in water as well as in oil. It can be prepared by combining the Pdop particle-mediated superhydrophilic mesh and superhydrophobic sponge composites. The self-floating all-in-one device simultaneously exhibits excellent removal performance for heavy metal ions in the water layer and excellent separation efficiency of oil in the oil layer due to its amphiprotic nature.

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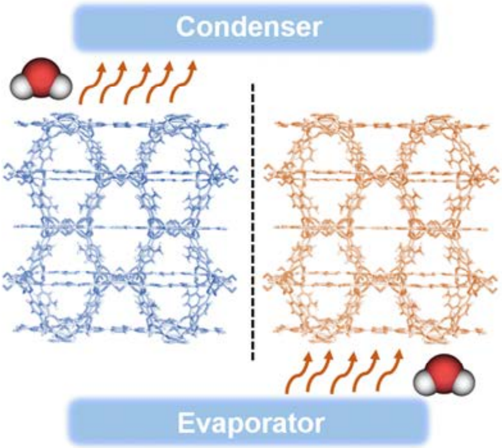
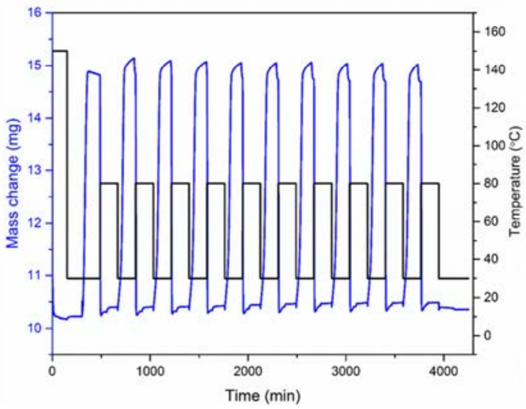
Synthesis of Highly Crystalline NH_2-MIL-125 with S-Shaped Water Isotherms

Muhammad Sohail 김태우[1] 김현욱[1,*]

과학기술연합대학원대학교(UST) 신에너지 및 시스템기술 [1]한국에너지기술연구원 에너지소재 연구실

Metal-Organic Frameworks (MOFs) have attracted attention for its application in the water-based heat transformation system. Herein, we report the synthesis of highly crystalline NH_2-MIL-125(Ti) material by two metal precursors such as Ti(*i*PrO)$_4$ and Ti(BuO)$_4$. Both products show an “S”-shaped water adsorption isotherm, but Ti(BuO)$_4$-derived NH_2-MIL-125 shows higher water capacity (0.68 g/g) than that (0.44 g/g) of Ti(*i*PrO)$_4$-derived one regardless of the synthesis method. In a sense of crystallinity, a solvothermal method with static conditions generated more distinct crystalline properties than the one synthesized by a reflux reaction as confirmed from PXRD analysis, UV–vis absorbance spectra and SEM images. Considering it as an adsorbent for the water-based heat transformation system, Ti(BuO)$_4$-derived sample synthesized by a solvothermal method shows an ideal S-shaped isotherm with a steep rise of water uptake at lower relative pressure (0.550 g/g at P/P_0 = 0.30), which is attributed to narrow triangle apertures and hydrophilic functional groups. This material shows the dynamic water adsorption/desorption cycle without any noticeable weight change. Details of the work will be presented.


Condenser
Evaporator


Mass change (mg)
Temperature (°C)
Time (min)
10
11
12
13
14
15
16
0
20
40
60
80
100
120
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2000
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4000

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나노다이아몬드를 포함한 중합체의 고기능성 레진 접합제로의 응용

이민제 김득현 정휘수[1] 성아영[*]

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나노다이아몬드는 우수한 경도뿐만 아니라 인체 내에서도 변하지 않는 특성과 무해한 특성을 가지고 있어 인공망막이나 약물 운송 장치 등의 바이오 의료장치에 사용되고 있다. 특히, 나노다이아몬드는 고분자 물질의 인장강도를 높여 레진 시멘트의 접착력과 강도를 증가시키는 역할이 가능하다. 본 연구는 나노다이아몬드를 첨가제로 사용하여 전단 및 굴곡강도 등을 증가시켜 우수한 치과용 접합시멘트를 제조하였다. 실험을 위해 Bis-GMA 그리고 HPMA 및 HEMA 등을 12 시간 이상 교반하고 희석제를 첨가한 후 30 분 이상 교반하였다. 또한 촉매제인 BPO 및 BHT 를 각각의 비율로 첨가 후 30 분 교반하였다. 강도를 증가시키기 위한 나노다이아몬드를 첨가하기 위해 약 40 분 이상 교반 하였다. 또한 460nm 파장에서 20 초 동안 광중합 하여 치과용 레진접합제를 제조하였다. 독성평가 결과 모든 조합에서 적합 하였다. 또한 전단결합강도 측정결과 나노다이아몬드를 첨가하지 않은 조합보다 전단결합강도가 높게 측정되었다. 특히, HpND 의 경우 전단결합 강도가 약 5.61~6.51 Mpa 로 측정되어 고 강도용 레진 접합제가 개발되었다.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-335**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Roles of Small Organic Molecules in Stabilizing Spherical Nucleic Acids (SNAs)

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Spherical nucleic acids (SNAs) have been intensively investigated owing to their unique chemical and physical properties such as programmable assembly, high binding affinity, and multifunctionality. In particular, SNAs have been widely utilized as smart probes for detecting a variety of targets with higher sensitivity and selectivity than conventional detection systems. Owing to the nature of the nucleic acids including their ability to form hydrogen bonding, however, the target-binding properties of the SNA probes are unexpectedly, yet sensitively affected by a change in pH of reaction mixtures. Although the pH of the reaction mixtures could be maintained to be almost consistent under buffer conditions, the failure of maintaining the same pH leads to a significant change in binding properties of SNAs. To address this issue, we have investigated the fundamental interactions of SNAs with pyridine and its derivatives, and report that, in fact, just the pH increase induced by pyridine is practically the only parameter accounting for pyridine's DNA-stabilizing effects under acidic conditions. Importantly, we prove that pyridine does not increase the Tm of hybridized SNAs even under acidic conditions, if the pH increase by pyridine is corrected to maintain the same initial pH.

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Investigation on $NaNO_3$-promoted CdO as CO_2 absorbent

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For reduction of CO_2 emission to atmosphere, many kinds of mid- and high-temperature CO_2 absorbents have been researched and developed. But, most researches on mid- and high-temperatures CO_2 absorbents were usually based on main group elements such as MgO, Mg–based absorbents, Ca–based absorbents and Li–based absorbents. However, in this paper, we focus on transition metal based material, CdO, as a mid temperature CO_2 absorbent. CdO itself doesn't show any CO_2 absorption, so we put $NaNO_3$ into CdO system for promoting CO_2 absorption and desorption. Up to 78% of CdO conversion efficiency was achieved, although the absorption ability decreased as the absorbent was used repeatedly in cycle, due to the growth of particles in size. For investigation on the growth of particle size, several analyses were conducted. Herein, we found that dissolution of CdO and $CdCO_3$ in molten $NaNO_3$ is necessary in respect of facilitating CO_2 absorption and desorption.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Adsorption and Removal of Pharmaceuticals and Personal Care Products from Water with Functionalized Metal-organic Frameworks: Remarkable Adsorbents with Hydrogen-bonding Abilities

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Typical pharmaceuticals and personal care products (PPCPs) (such as naproxen, ibuprofen and oxybenzone) were adsorbed from aqueous solutions on highly porous metal-organic framework (MOF) MIL-101 with and without functionalization. Adsorption results showed that MIL-101s with H-donor functional groups such as –OH and –NH2 were very effective for naproxen adsorption, despite a decrease in porosity, probably because of H-bonding between O atoms on naproxen and H atoms on the adsorbent. For this reason, MIL-101 with two functional groups capable of H-bonding (MIL-101-(OH)2) exhibited remarkable adsorption capacity based on adsorbent surface area. The favorable contributions of –OH and –(OH)2 on MIL-101 in the increased adsorption of ibuprofen and oxybenzone (especially based on porosity) confirmed again the importance of H-bonding mechanism. The adsorbent with the highest adsorption capacity, MIL-101-OH, was very competitive when compared with carbonaceous materials, mesoporous materials, and pristine MIL-101. Moreover, the MIL-101-OH could be recycled several times by simply washing with ethanol, suggesting potential application in the adsorptive removal of PPCPs from water.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Adsorption and Removal of Artificial Sweeteners from Water Using Metal-Organic Frameworks Functionalized with Urea or Melamine

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Urea or melamine was introduced into a highly porous metal-organic framework (MOF), MIL-101, via grafting on open metal sites of the MOF. Adsorptive removal of three artificial sweeteners (ASWs) was studied using the MOFs, with or without modifications (including nitration), and activated carbon (AC). The adsorbed quantities (based on the weight of the adsorbent) of saccharin (SAC) under various conditions decreased in the order urea-MIL-101 > melamine-MIL-101 > MIL-101 > AC > O2N-MIL-101; however, the quantities based on unit surface area are in the order melamine-MIL-101 > urea-MIL-101 > MIL-101 > O2N-MIL-101. Similar ASWs [acesulfame (ACE) and cyclamate (CYC)] showed the same tendency. The mechanism for very favorable adsorption of SAC, ACE, and CYC over urea- and melamine-MIL-101 could be explained by H-bonding on the basis of the contents of –NH2 groups on the MOFs and the adsorption results under a wide range of pH values. Moreover, the direction of H-bonding could be clearly defined (H acceptor: ASWs; H donor: MOFs). Urea-MIL-101 and melamine-MIL-101 could be suggested as competitive adsorbents for organic contaminants (such as ASWs) with electronegative atoms, considering their high adsorption capacity (for example, urea-MIL-101 had 2.3 times the SAC adsorption of AC) and ready regeneration.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Metal–Organic Framework UiO-66 with Free Carboxylic Acid: Versatile Adsorbents for Both Aqueous and Non-aqueous Phase

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Zirconium chloride and isophthalic acid (IPA), together with the usual terephthalic acid (TPA), were converted into the metal–organic framework (MOF) UiO-66 in one step. 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 (adsorbates: H donor; MOFs: H acceptor) 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.

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장소: 일산 KINTEX
발표코드: **MAT.P-340**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Adsorption and removal of organic sulfur- and nitrogen-containing aromatics from fuel with with scandium-triflate/metal-organic frameworks

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Benzothiophene (BT), dibenzothiophene (DBT), quinoline (QUI) and indole (IND) are the most common organic sulfur- and nitrogen-containing aromatics that exist in liquid fuel as contaminant. These compounds should be removed prior to utilization of liquif fuel in various means. 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.

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장소: 일산 KINTEX
발표코드: **MAT.P-341**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Hydrophobicity/hydrophilicity of adsorbents and solvent polarity effect on liquid-phase adsorption of aromatics over a metal–organic framework and activated carbon

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Hydrophilicity/hydrophobicity of adsorbents and solvent polarity are effective parameters for the adsorption aromatics which were investigated via liquid phase adsorption over a metal-organic framework (MOF, MIL-101) and activated carbon (AC). Aromatics having low acidity or basicity, such as thiophene, pyrrole, and nitrobenzene were selected as adsorbates for this study. Adsorption tests were carried out for selected adsorbates over MIL-101 and AC to estimate possible applications of the adsorbents in liquid-phase adsorptions the adsorbents in adsorptive desulfurization (ADS), adsorptive denitrogenation (ADN), and water purification, respectively. With decreasing the solvent polarity, MIL-101 adsorbed all the three adsorbates more effectively than AC and the reverse was observed for AC. Analyses of hydrophobicity indexes for MIL-101 and AC revealed with the effect of the hydrophilicity of MIL-101 and hydrophobicity of AC on the adsorption of tested sorbates. The superior 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 more effective than hydrophobic AC. Finally, it is necessary to increase the hydrophobicity of a MOF for the adsorptions of aromatics from water, to explain the applicability of MOFs in water purification.

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장소: 일산 KINTEX
발표코드: **MAT.P-342**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Adsorptive removal of benzotriazole and benzimidazole from water over a Co-based metal azolate framework

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Co-based metal azolate framework, MAF-5(Co) has been used in the water purification for the removal of toxic water pollutant, benzotriazole (BTA) and benzimidazole (BZI) from aqueous solution. The adsorption capacity of the MAF-5(Co) for BTA and BZI was highest than that of commercial activated carbon or other typical adsorbents including metal–organic frameworks (MOFs). Hydrophobic and π-π interactions between the BTA and MAF-5(Co) were suggested as a plausible mechanism. Based on the zeta potential of MAF-5(Co) and effects of pH on the BTA adsorption, electrostatic interactions between the MAF-5(Co) and BTA species might also affect the adsorption of BTA over MAF-5(Co). Moreover, MAF-5(Co) can be recycled for adsorptive removal of BTA by simple ethanol treatment. Therefore, MAF-5(Co) can be suggested as an efficient adsorbent for BTA and BZI removal from water considering the highest adsorption capacity, excellent reusability, and facile synthesis.

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장소: 일산 KINTEX
발표코드: **MAT.P-343**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

CO_2 absorption and desorption mechanisms of A_2CO_3-promoted MgO (A=Na, K, Rb, Cs)

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CO_2 capture and sequestration (CCS) is regarded as a key technology for reducing CO_2 emission from power plants based on fossil fuel. Among the various CO_2 absorbents, MgO is a possible candidate in intermediate-temperature (200-500 ^oC) range because of low decomposition temperature from carbonate ($MgCO_3$) into oxide among other alkali and alkaline earth metal carbonate. The theoretical CO_2 absorption capacity of MgO is highest among the other absorbents, but sluggish absorption kinetics makes its application hard. In order to overcome this sluggish kinetics, alkali metal carbonates have been suggested for enhancing the reactivity of MgO with CO_2. Promoting mechanism was already discussed by previous researchers but their explanation was not sufficient. Here, we suggest developed CO_2 absorption and desorption mechanisms of alkali metal carbonates promoted-MgO. Pretreatment effect before CO_2 absorption of absorbents is evaluated by ^{23}Na and ^{25}Mg solid state MAS NMR analysis. At the superbase sites in the lattice of MgO, MgO can react with CO_2 and $MgCO_3$ can be formed. After that, $A_2Mg(CO_3)_2$ is formed by interfacial diffusion between A_2CO_3 and $MgCO_3$. CO_2 desorption is the reverse reaction of CO_2 absorption. Detailed data will be presented in the poster section.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-344**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Determination of Binding Properties of Spherical Nucleic Acids by Constructing Multicomponent Layers

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Spherical Nucleic Acids (SNAs) have been employed in various applications such as building blocks for nano-architecture, drug carriers for intercellular delivery, multifunctional probes for biological target detection, and heat-radiating agents for photothermal therapy, based on their selective and sensitive binding properties. For this reason, controlling binding properties of SNAs is one of the most significant subjects to achieve the aforementioned goals. Typically, the construction of multicomponent layers employing non-reactive chemicals, i.e. diluents, is widely devised, but further systematic examination of the nanoparticle-conjugation conditions needs to be thoroughly carried out. In this presentation, we observe that non-reactive diluents exhibit more complicated interfacial interactions and eventually control overall conjugation of ligands to the core nanoparticles. Furthermore, we demonstrate what exactly controls the construction of a bicomponent layer on nanoparticle surfaces, and how the overall binding properties of the SNAs can be controlled, providing strong and general guidelines for the preparation of SNAs.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-345**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Sodium Storage Property of WSe_2 with Different Particle Size and Irradiation Dose

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Sodium ion battery was expected to be a next-generation battery that can replace lithium-ion battery because sodium is abundant in deposit and has a physicochemical similarity with lithium. However, since the radius of the sodium ion (0.106 nm) is larger than the radius of the lithium ion (0.076 nm), it is necessary to experience rapid volume change and capacity reduction during the charging/discharging process. Therefore, to develop a sodium ion battery with improved electrochemical performance, a new strategy must be attempted. Systematic research on developing local disorder at WSe_2 was carried out to obtain enhanced sodium storage property. By adopting mechanical method, exfoliated WSe_2 and its self-restacked form were successfully synthesized. The synthesized WSe_2 nanosheets with different particle sizes were further treated by ion beam. The shapes of restacked layers were characterized from scanning electron microscopy while developed local disorders were confirmed from changes in EXAFS and Raman. Changes in electrochemical properties such as cyclabilities and specific capacities were probed from the charge/discharge experiments.

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장소: 일산 KINTEX
발표코드: **MAT.P-346**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of NiO/graphene Hybrid with Enhanced Energy Storage Property

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Metal oxides with a higher capacity than graphene-based materials have actively studied as an anode material. However, they had inherent limitations such as a large volume change and low electrical conductivity. To overcome such drawbacks, the NiO/GO hybrid was synthesized through two step process: hydrothermal synthesis and subsequent heat treatment. The physicochemical properties are characterized by XRD, SEM, TEM, FT-IR, RAMAN and BET analysis. The TEM image showed that nanosized NiO particle with a hexagonal morphology was attached on the graphene nanosheets, indicating the interaction between the NiO and the graphene sheet. According to galvanostatic discharge/charge, the NiO/graphene hybrid had superior capacity and high rate capability in sodium storage due to the complementary synergy effect between the NiO nanoparticle and the graphene nanosheet. It is expected that this hybrid could be widely utilized as active material for advanced energy system storage.

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발표코드: **MAT.P-347**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A palladium-based metallomesogen for an optoelectronical tunable polarized light modulator

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A photo-responsive metallomesogen containing azobenzene (abbreviated as PRM) was synthesized to fabricate an optically and electrically tunable polarized light modulator. On basis of diffraction results with thermal and morphological ones, it was found that PRM formed a highly ordered smectic crystal phase. In addition, PRM showed excellent solubility in LC media. For polarized light modulator, PRM-filled IPS cell is fabricated and characterized. Reorientation direction of PRM induced by the in-plane electric field made absorption intensity of the polarized light high. When aligned direction of PRM is parallel with the polarized direction of light, the absorbance is increased. Furthermore, the absorption properties of PRM-doped optical cell is changed depending on wavelengths of the light. Because of azobenzene, the alignment of PRM break under ultra-violet irradiation. It makes the adsorption intensity low. Under visible light, the alignment of PRM return and the adsorption intensity is increased. This work was supported by the MOTIE/KDRC 10051334, BK21 Plus program, Mid-Career Researcher Program (2016R1A2B2011041).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-348**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Effect of Amine-Functionalization on Acid-Treated Halloysite Nanotubes for Adsorption of Eosin Y

이형욱 이건구 노재근*

한양대학교 화학과

Halloysite nanotubes (HNTs), tubular clay mineral, are naturally occurring clay mineral. Pristine halloysite nanotubes (HNTs) were pretreated to produce acid treated halloysite nanotubes which have enlarge pore and surface area. Amine-functionalized HNTs (A-HNTs) were prepared after surface modification of acid-treated HNTs by 3-aminopropyltriethoxysilane, which can be used as an adsorbent for 2-(2,4,5,7-tetrabromo-6-oxido-3-oxo-3H-xanthen-9-yl)benzoate) [eosin Y] that is most commonly used as an acidic red stain. The dye is also not specifically listed as a toxic substance by different health agencies. Because of its stability, non-toxicity and complex aromatic structure, eosin Y is used in the fields of leather, printing, dyeing, printing ink, fluorescent pigment, photo-photocatalyst, and so on. We compared the corresponding adsorption capacity of acid treated HNTs and A-HNTs. Characteristics of prepared A-HNTs were examined by mean of the Brunauer−Emmett−Teller (BET), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), and ultraviolet–visible spectroscopy.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-349**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Intercalation of Halloysite Nanotubes by Sodium Acetate and Dimethyl Sulfoxide and Their Adsorption Ability for Dye Molecules

이건구 이형욱 노재근*

한양대학교 화학과

Halloysites have multi-walled nanotubes with an interlayer spacing of 10 Å that can be used for various applications, such as, additives in polymers and plastic, electronic components, drug delivery vehicles, adsorption of toxic compounds in water, and cosmetics. In this study, to enhance the adsorption ability of holloysite nanotubes (HNTs), we try to widen the interlayer spacing of HNTs by the insertion of a guest species in the interlayer region of HNTs with preservation of the layered structure, which is called intercalation. HNTs were intercalated by sodium acetate (SA_HNTs) and dimethyl sulfoxide (DMSO_HNTs). SA_HNTs were intercalated resulting from electrostatic repulsion in interlayers and DMSO_HNTs were intercalated by new hydrogen bonding with S=O groups and hydroxyl group of interlayers. It is expected that the intercalated HNTs significantly affect the adsorption of dye molecues (Methylene Blue) because the spacing of interlayers was widened. Intercalation and adsorption ability of HNTS for dye molecules were characterized by Fourier transformed infrared spectroscopy (FT-IR), Ultraviolet-visible spectroscopy (UV), X-ray diffraction (XRD), and Brunauer-Emmett-Teller (BET). FT-IR measurements demonstrated that the intercalation of HNTs was confirmed by the presence of C=O vibration peak at 1420 cm-1 and S=O vibration peak at 1043 cm−1. From UV measurements, raw_HNTs, SA_HNTs and DMSO_HNTs show significant difference in adsorption of dye molecules. We found that the intercalated HNTs for adsorption of dye molecules are more effective than raw_HNTS.

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발표분야: 재료화학
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A new hollow nanostructures between titanate and graphene oxide for enhanced sodium-ion storage performance

이원재 백승민*

경북대학교 화학과

Recently, in the field of energy storage system, the sodium-ion batteries (SIBs) have highly been attracted research interests in the both scientific and industrial fields because of natural abundance and cost-effective property of sodium. In this study, the new hollow nanostructures between titanate and graphene oxide were successfully synthesized via chemical exfoliation and layer-by-layer self-restacking technique, and then, the product was used as an anodic material of SIBs. The spherical hollow structures were observed in the electron microscopy analysis such as SEM and TEM. According to energy dispersive spectroscopy mapping, the carbon and titanium atoms were homogeneously distributed in samples. The half-cell test shows that the synthesized product could be used as a anodic materials for SIBs with enhanced performance.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-351**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Pd-decorated on CNTs as highly efficient catalysts for the reduction of aromatic nitro compounds

김지당 최현철*

전남대학교 화학과

Aromatic nitro compounds are the pollutants in wastewater. Pd-based compounds have high catalytic activity for the reduction of aromatic nitro compounds. By the way, the applications of Pd nanoparticles remain limited by weakness in terms of their easy aggregation and the difficulty of catalyst product separation. In this study, we synthesized Pd-decorated CNT by introducing thiol groups on CNTs. The thiol of surface modification is an effective way to obtain dispersed metal nanoparticles on the surface of CNT. We have successfully simple prepared CNT-Pd nanocomposites with a reduction of Pd (II) ions. To study the catalytic activity, a 1 x 10-3 M of aqueous aromatic nitro compounds solution was mixed with 0.1 M of fresh NaBH4 solution. CNT-Pd catalysts were added and stirred. The mixture was immediately transferred into a quartz cuvette and UV-vis absorption spectra were recorded to monitor changes in the reaction mixture. The samples were characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and transmission electron microscopy (TEM). The reduction kinetics of aromatic nitro compounds is also investigated by ultraviolet-visible (UV-vis) measurement.

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Synthesis of GeH and $GeCH_3$ and its application to Li and Na ion battery

강민경 김성진[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학과

Germanium has been considered as a promising anode material because of its comparable lithium and sodium storage capability and fast Li diffusivity. Nevertheless, despite the huge capacity, it exhibits poor cycling stability due to the drastic volume change during the lithium or sodium uptake and release processes, leading to structural damage and capacity fading. To improve the cycle performance, two-dimensional (2D) materials with weak interaction between the layers have been proposed as promising anodes in Li-ion batteries because the structural damage by large volume variation could be decreased due to stretching vertically between layers instead of volume change to all directions. Here we show that germanane (GeH) and methyl-terminated germanane ($GeCH_3$) made from calcium germanide ($CaGe_2$) can be used as promising anodes for Li and Na ion batteries. The germanane (GeH) and methyl-terminated germanane ($GeCH_3$) were synthesized using by solid state reaction. The crystal structures of the sample were analyzed by X-ray diffraction (XRD) and RAMAN spectrum. The batteries of germanane (GeH) and methyl-terminated germanane ($GeCH_3$) were tested as high capacity anodes in lithium ion (Li-ion) batteries using Wonatech WBCS3000S battery test system.

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Synthesis and thermoelectrical properties ofSulfur-doped $CuBi_2O_4$

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Thermoelectric materials attract vast attention due to the present energetic and environmental needs for new potential renewable energy source. The dimensionless figure of merit, ZT, is the key parameter that defines the efficiency of thermoelectric materials. The *ZT* value, $(S^2\sigma/\kappa)T$, is derived from thermal conductivity (κ), electrical conductivity (σ) and Seebeck coefficient (S) with Temperature T. Thermoelectric oxides have been widely investigated over the past decades owing to their nontoxicity, low cost, and thermal and chemical stability in air. Among the various kinds of thermoelectric oxide materials, spinel $CuBi_2O_4$ is a promising new oxide thermoelectric material with band gap of 1.5-1.8 eV. In this study, $CuBi_2O_4$ was synthesized through solid state reaction. Sulfur-doped $CuBi_2O_4$ was prepared by sulfurization using CS_2 gas. Comparative investigations of the $CuBi_2O_4$ and sulfur-doped $CuBi_2O_4$ system were performed to have a better understanding for the effect of sulfurization of $CuBi_2O_4$ on the thermoelectric properties. The crystal structure and thermoelectric properties such as Seebeck coefficient and thermal conductivity of prepared samples were measured with X-ray diffraction, ZEM-3 equipment (Ulvac-Riko), and NETZSCH LFA 457 MicroFlash™. The X-ray diffraction data indicates that the structure of $CuBi_2O_4$ was remained after the substitution of sulfur. The ZT value of sulfur-doped $CuBi_2O_4$ was 1.4*10-3 at 400K. The substitution of O site by S provides possible directions toward the enhancement of the thermoelectric figure of merit of oxide materials with low electrical conductivity.

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발표분야: 재료화학
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Synthesis and Thermoelectric Properties of Cu2-xSe and CuAgSe

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The thermoelectric (TE) energy conversion technology has received much attention in the past decades. It has a potential impact on efficient world–wide energy harvesting. The theoretical maximum conversion efficiency is defined by $\eta = \surd(1+ZT)$, where ZT is the dimensionless parameter known as the figure of merit: $ZT = S2\sigma T/\kappa$. An ideal TE material should have a high power factor (S2s) as well as low thermal conductivity (κ). However, because of the interrelation between transport parameters, it is very challenging to achieve high ZT values. Recently, superionic conductors with the concept of the "phonon-liquid electron-crystal (PLEC)" has been used to abnormal but attractive. The binary Cu2-xSe and ternary CuAgSe are kind of superionic conductor that agrees well with PLEC concept. In this study, we tried to synthesize uniform sized surfactant-free Cu2-xSe nanoplates and nanowires and CuAgSe nanoparticles. We found that the size and morphology can be controlled by changing the reaction time and solution concentration. We consolidated Cu2-xSe and CuAgSe nanoparticle to bulk pellet via a simple route, spark plasma sintering (SPS). As a consequence, ZT value of Cu2-xSe continuously increase, but CuAgSe shows high ZT value at low temperature. The maximum ZT value for Cu2-xSe is 0.27 at 723 K, whereas, CuAgSe is 0.59 at 323K.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Study of CO_2 adsorption on alkali metal and alkaline earth metal surface treated activated carbon

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계명대학교 화학과

Activated carbon was treated with alkali metal by addition of Lewis acid catalyst at room temperature. Surface treated alkali metals are present on the surface of activated carbon in the form of MOH or MO (M= alkali metal and alkaline earth metal), which is thermodynamically highly reactive with CO_2. Because it exists in a stable carbonate form while reacting with an metal oxide or an metal hydroxide. The specific surface area of the surface-treated activated carbon was confirmed by N_2-sorption. Chemical binding state of alkali metal were charaterized using SEM-EDS, EPMA and XPS. Surface treated activated carbon with alkali metal as sorbent showed to improve CO_2 adsorb performances at room temperature.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High reduction rate of graphene oxide via controlled reflux time in dimethylformamide

장다운 박성진[1,*]

인하대학교 자연과학부/화학과 [1]인하대학교 화학과

The reduction of graphene oxide (G-O) is the most widely used methods for the large scale production of graphene-based materials. In this paper, we report a simple and environmentally-friendly method to produce reduced graphene oxide (rG-O) by refluxing G-O in N, N-dimethylformamide without using a reducing agent. The rG-O materials with high degrees of reduction are prepared and the levels of reduction are controlled using reflux time. Successful reduction is confirmed by combustion-based elemental analysis and X-ray photoelectron and Fourier transform infrared spectroscopy.

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발표분야: 재료화학
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Cs2SnI6-based Hole Transporting System Generating High Photocurrent Density for Dye-sensitized Solar Cells

신현오 권태혁[1,*]

UNIST 화학과 [1]UNIST 친환경에너지 공학부

Pb-based perovskite has attracted a great attention as the multifunctional materials in next generation solar cells because of great light harvesting ability, ambipolar conductance, etc. However, despite of their brilliant properties, the toxicity of centered atom has limited their application to broad field and triggered the researches on Pb-free perovskite. As the representative of the Pb-free perovskite, Cs2SnI6 perovskite is stable in ambient conditions and showed the great ability as the hole transport material in the dye-sensitized solar cells (DSSCs). In this work, we suggest the efficient hole transporting system(HTS) that is consisted of Cs2SnI6 perovskite and ionic liquid (DMPII) in succinonitrile. We also investigate their compatibility with various sensitizers in terms of thermodynamic energy level. In such Cs2SnI6-based HTS, Cs2SnI6 showed faster charge transfer rate compared with general iodine couples and DMPII compensated the high viscosity of succinonitrile medium. Due to their complementary cooperation, BT-T2 DSSC based on Cs2SnI6-based HTS generated much higher photocurrent density than conventional liquid-type DSCs with iodine. Consequently, we achieved 5.5% of power conversion efficiency with only 1.8-μm thin TiO2 film, which was higher than the best one of liquid-type BT-T2 DSSC. We studied the conductivity and charge transfer resistance in Cs2SnI6-based HTS using several electrochemical analyses. Moreover, from TCSPC and IMPS&VS analysis, we revealed Cs2SnI6-based HTS showed higher regeneration efficiency and charge collection efficiency compared with iodine electrolyte. This work demonstrated the excellence of the Pb-free perovskite compared with iodine electrolyte, contributing the growth of further researches on Pb-free perovskite and DSSCs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-358**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Cu(Ⅱ)-bpy based POPs : an efficient catalyst for epoxidation

이지경 이석중*

고려대학교 화학과

Recently, epoxidation has attracted much attention because it is the most effective method for carbon-oxygen bonding formation. Among various available transition metal, copper is most suitable material due to not only economic point of view but higher reduction potential. Currently, much studies have been made to heterogenize homogeneous catalysts by integrating them into porous materials like porous organic polymers (POPs), covalent organic frameworks (COFs), polymers of intrinsic microporosity (PIM). These materials have many advantage of recycling, recovery, and site isolation. In this regard, we have prepared POPs that are composed with bipyridine and *tetrakis*(4-ethynylphenyl)methane using a cobalt catalyzed acetylene trimerization reaction. The resulting POPs were metalated with CuCl$_2$ followed and were carried out olefin oxidation. Detailed structures and other measurement will be given in the presentation.

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장소: 일산 KINTEX
발표코드: **MAT.P-359**
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Selective ethylene dimerization using novel Ni(Ⅱ)-bpy based POP as heterogeneous catalyst

<u>김민정</u> 이석중*

고려대학교 화학과

Recently, increasing attention has been drawn to porous materials such as metal-organic frameworks (MOFs), porous organic polymers (POPs), and covalent organic frameworks (COFs) from both the academic and the industrial communities. Because, they have outstanding properties such as high porosity and have been used as catalysis, gas storage, and separation of molecules. Especially, Heterogeneous catalysis is widely studied alternative to homogeneous catalysis due to its advantages which are facile separation, recyclability. MOFs are the most widely used in heterogenizing homogeneous catalysts. But POPs are focused on new opportunities for heterogeneous catalysis due to its thermally and chemically stability, low cost and easy to make. Therefore, we have synthesized a POP-1 with 'click-reaction' via strong copper-catalyzed alkyne–azide coupling (CuAAC). POP-1 is based on bipyridine ligand for providing metal site to metalation with nickel for ethylene dimerization reaction. In this presentation. We like to show our model of POP-1 and paramount challenge about controlling the selectivity about the product 1-butene which is required in high purity for application as a comonomer in polyolefin.

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일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT.P-360**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and Characterization of White-Light Emitting Nanohybrid Material Based on Clay

김아란 정 현*

동국대학교 화학과

White-light emitting solid materials have attracted significant attention due to their broad applications in optoelectronic devices, such as full color displays and the solid-state lighting. In this work, we have prepared white-light emitting nanohybrid material composed of rhodamine 6G (R6G) and 2,5-bis(5-tert-butyl-benzoxazol-2-yl)thiophene (BBOT) based on clay (Laponite XLG) within a transparent polymer matrix. Organic dye molecules adsorb on the clay surface through the electrostatic interaction between cationic dye and clay layer. The resulting hybrid has been characterized by powder X-ray diffraction (XRD), and fluorescence spectroscopy. We observed white-light emission in the solid-state at room temperature.

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장소: 일산 KINTEX
발표코드: **MAT.P-361**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Nitrogen-doped mesoporous graphene with controlled pore sizes for high-performance supercapacitors

이지혜 정 현*

동국대학교 화학과

Nitrogen-doped mesoporous graphene (NMG) with interpenetrating porous network was successfully synthesized and their pore size was tuned by controlling the volume ratio of washing solvent. As-prepared NMG was synthesized by hydrothermal process of graphite oxide (GO), self-assembled amphiphilic triblock copolymer (Pluronic P123), and ammonium hydroxide, wherein P123 and ammonium hydroxide was used as soft-template and nitrogen source, respectively. And then, as-prepared NMG was washed with the various volume ratios of water to ethanol. Finally, the obtained products were sintered under Ar atmosphere. The synthesized NMGs have high BET specific surface area (941 – 1198 m^2/g) and narrow mesopore size distribution. Furthermore, average mesopore size of NMG can be rationally controlled by regulating the volume ratio of water to ethanol. With the increase of ethanol ratio, the average mesopore size is decreased to be from ~11.2 nm to ~4.4 nm. In order to determine supercapacitor capacitance, cyclic voltammetry curves and galvanostatic charge-discharge tests were performed in a three-electrode system in 6 M KOH. In addition, supercapacitor capacitance of NMGs had been compared with mesoporous graphene (MG) and nitrogen-doped graphene (NG).

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발표코드: **MAT.P-362**
발표분야: 재료화학
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Synthesis and characterization of pore size tailored mesoporous graphene

Rosalynn Nankya 이지혜 정 현*

동국대학교 화학과

Mesoporous graphene (MG) with tailored pore size was successfully synthesized by three distinctive synthesis processes using soft-template method. First method involved freeze drying of composite gel of graphite oxide (GO) and self-assembled triblock co-polymer (P-123). The second method was performed by hydrothermal treatment of the composite mixed solution. Third method included the addition of sodium hydroxide as a base catalyst to second method. And then, all of the obtained samples were sintered at 700 ^{o}C for 3 h under Ar atmosphere. The obtained samples after sintering were denoted as f-MG, h-MG, and h-MG-C, respectively. The synthesized samples were characterized by measurement of X-ray diffraction (XRD), Raman spectroscopy, field emission scanning electron microscope (FE-SEM), high resolution transmission electron microscope (HR-TEM), and elemental analysis. The f-MG, h-MG and h-MG-C have average mesopore size of 11.2, 5.0, and 3.9 nm with approximately full width half maximum (FWHM) values of 17, 7, and 3 nm, respectively by N_2-adsorption-desorption isotherm measurements. In case of the hydrothermal method, obtained samples exhibited the narrow pore distribution. Especially that which involved base catalyst showed the narrowest pore size distribution, which might be due to formation of covalent ester bonds between the graphite oxide layers caused by the base catalyst.

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발표코드: **MAT.P-363**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

One-pot synthesis route for the production of Pd nanoparticles and MWCNTs-supported Pd-nanomaterial composites

송재희

순천대학교 화학과

We present a synthesis route for the production of Pd nanoparticles and MWCNTs-supported Pd composites by a simple proton beam irradiation process in an aqueous solution at room temperature. Pristine and thiolated 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 successfully controlled. 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.

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One-step immersion-based facile fabrication of Au nanoparticle films onto diverse substrate for bioassay platforms

김정효 오상진[1] 정기재[1] 이재범[2,*]

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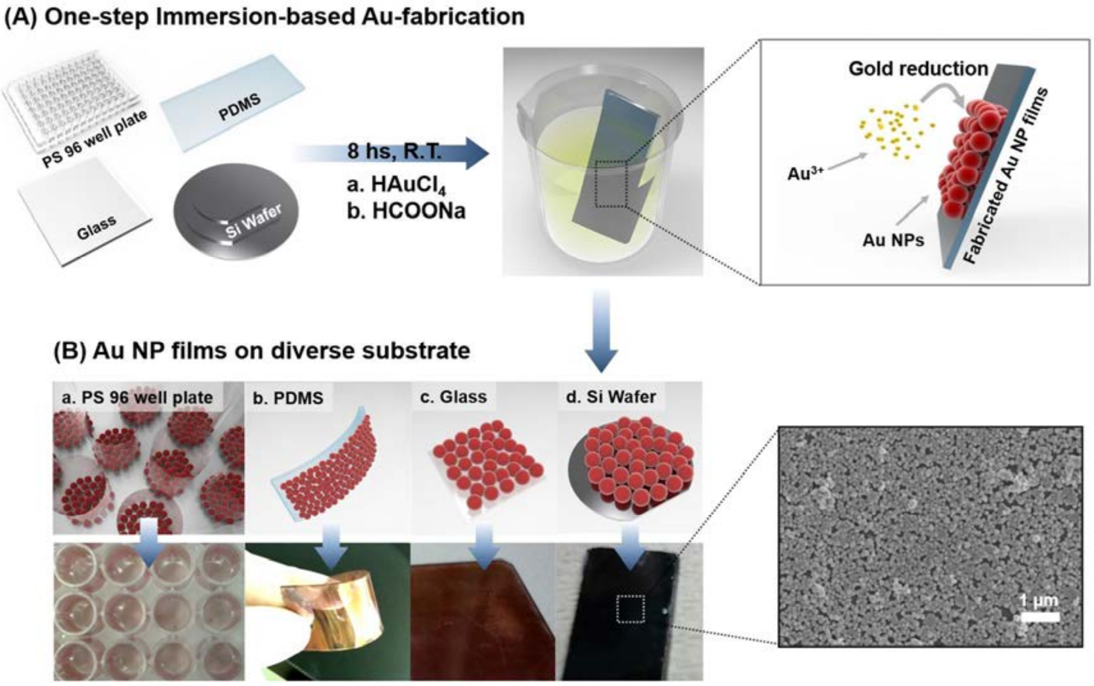
Nanomaterials without chemical linking or physical interaction resided on two-dimensional surface have been attractive due to their unique quantum confinement properties and further electronics and biomedical applicability. An in situ method has been developed to fabricate gold nanoparticle (NP) films on different substrates regardless of hydrophilic or hydrophobic surfaces, including glass, 96 polystyrene well plates, and polydimethylsiloxane (PDMS). A mixture of HCOONa and HAuCl4 solution was used to obtain Au NP films at room temperature on the hydrophilic and hydrophobic surfaces. Experimental study of the mechanism revealed that film formation is dependent on surface wettability. The surface-enhanced Raman scattering enhancement grew stronger on films obtained with solutions containing increasing sodium formate (HCOONa) concentrations. The as-fabricated Au NP films were also used to successfully bind antibodies to check their applicability in bioassays.


(A) One-step Immersion-based Au-fabrication

(B) Au NP films on diverse substrate

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장소: 일산 KINTEX
발표코드: **MAT.P-365**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Triphenylene-based Heat Transfer Reactive Dicogens

임석인 구자현 정광운[1,*]

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Since the amount of heat accumulation is proportional to the power density, the effective heat management is important to improve the reliability and lifetime of devices. For the fabrication of advanced heat transfer organic materials, we synthesized triphenylene-based reactive discogens 2,3,6,7,10,11-hexakis(but-3-enyloxy)triphenylene (HBOTP) and 4,4′,4″,4‴,4⁗,4⁗′-(triphenylene-2,3,6,7,10,11-hexaylhexakis(oxy))hexakis(butane-1-thiol) (TPHBT) as discotic liquid crystal monomers and cross-linkers, respectively. Based on the temperature−composition phase diagram of HBOTP-TPHBT mixtures and the physical, chemical, and thermal properties of Triphynylene-based heat transfer reactive discogens(TP HTRDs), the optimum content of HBOTP was determined. the TP HTRDs were polymer-stabilized by UV-irradiation at 80 °C. The TP HTRDs with outstanding thermal conductivities as well as with excellent mechanical and chemical stabilities can be applied as heat dissipating materials in electronic, automobile, and display industries. This work was supported by the BK21 Plus, the BRL 2015042417, and Mid-Career Researcher Program (2016R1A2B2011041).

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Solution-Processable Emitting Materials for Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes (TADF-OLEDs)

최영빈 최동훈*

고려대학교 화학과

Recently, thermally activated delayed fluorescence (TADF) using both singlet (25%) and triplet (75%) excitons has attracted much interest as the most promising alternative for efficient OLEDs. In the field of OLED device processing, a solution process has been highlighted due to the simplified layer-deposition method, low-cost and large-area production unlike the well-known vacuum process. Despite these many advantages, there was a few study on the solution-process-based TADF-OLEDs. In this work, we designed and synthesized the solution-processable emitting materials for TADF-OLED device processing. The physical properties of the materials were characterized and the corresponding device characteristics such as turn-on voltage (Von), luminance (L) and external quantum efficiency (EQE) were also investigated by fabricating simple OLED devices.

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Promoting Oxygen Reduction Reaction Activity of Active-Site-Rich Fe−N/C Electrocatalysts by Silica Coating Strategy

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UNIST 화학공학과 [1]UNIST 화학과 [2]UNIST 에너지화학공학부

Oxygen reduction reaction (ORR) is an important half-reaction in clean energy conversion devices such as polymer electrolyte fuel cells (PEFCs). Sluggish reaction kinetics of the ORR renders the use of Pt-based electrocatalysts that are efficient; however, they are scarce and expensive, thus precluding the wide employment of PEFCs. Iron and nitrogen codoped carbon (Fe−N/C) catalysts have demonstrated promise as substitutes for the Pt-based catalysts due to their high ORR activity, which has been found to stem from the atomically dispersed Fe coordinated with nitrogen atoms (Fe−Nx site). Rational design that can create abundant active Fe−Nx site remains an important challenge in Fe−N/C catalysts. Recently, we have developed the silica-coating-assisted synthetic strategy for high-performance Fe−N/C catalysts using metalloporphyrin as Fe and N precursors. In this work, we generalize this synthetic concept with more affordable Fe and N precursors, such as iron acetate/1,10-phenanthroline and iron acetate/polyaniline. In addition, we extensively explored the impacts of pyrolysis temperature and Fe contents, and the type of carbon support on the ORR activity of the resulting Fe−N/C catalysts. The silica coating step during the preparation of Fe−N/C catalysts was generally effective to make the Fe−N/C catalysts predominantly composed of active Fe−Nx site while suppressing the generation of inactive Fe-based particles, thus significantly improving the ORR activity of the Fe−N/C catalysts. Significantly, the addition of S-containing precursor further boosted the ORR activity of Fe−N/C catalysts.

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Silica-Protective-Layer-Assisted Formation of Active Fe−N_x Sites in Fe−N/C Electrocatalysts for Efficient Oxygen Reduction Reaction

사영진 우진우[1] 주상훈[2,*]

UNIST 화학과 [1]UNIST 화학공학과 [2]UNIST 에너지화학공학부

Iron- and nitrogen-doped carbon (Fe−N/C) catalysts have emerged as promising nonprecious metal catalysts (NPMCs) for oxygen reduction reaction (ORR) in energy conversion and storage devices. It has been widely suggested that an active site structure for Fe−N/C catalysts contains Fe−N_x coordination. However, the preparation of high-performance Fe−N/C catalysts mostly involves a high-temperature pyrolysis step, which generates not only catalytically active Fe−N_x sites, but also less active large iron-based particles. In this presentation, we present a general “silica-protective-layer-assisted” approach that can preferentially generate the catalytically active Fe−N_x sites in Fe−N/C catalysts while suppressing the formation of less-active large Fe-based particles. The catalyst preparation consisted of an adsorption of iron porphyrin precursor on carbon nanotube (CNT), silica layer overcoating, high-temperature pyrolysis, and silica layer etching, which yielded CNTs coated with thin layer of porphyrinic carbon (CNT/PC) catalysts. Temperature-controlled in situ X-ray absorption spectroscopy during the preparation of CNT/PC catalyst revealed that the coordination of silica layer can stabilize the Fe−N_4 sites. The CNT/PC catalyst contained higher density of active Fe−N_x sites compared to the CNT/PC prepared without silica coating. The CNT/PC showed high ORR activity and excellent stability in alkaline media. Importantly, an alkaline anion exchange membrane fuel cell (AEMFC) with a CNT/PC-based cathode exhibited record high performances among NPMC-based AEMFCs. In addition, a CNT/PC-based cathode exhibited a high volumetric current density of 320 A cm^{-3} in acidic proton exchange membrane fuel cell.

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Metal-Support Interaction between Platinum and Mesoporous Molybdenum Carbide for Efficient Alkaline Hydrogen Evolution Reaction

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More sluggish reaction kinetics and inferior stability of Pt catalysts for alkaline hydrogen evolution reaction (HER) compared to acidic HER represent a great challenge in alkaline electrolyzer technologies, which is an essential element in sustainable hydrogen economy. In this presentation, we have synthesized mesostructured molybdenum carbide supported Pt (Pt/MMC) catalyst for alkaline HER, and demonstrate that the alkaline HER activity of Pt nanoparticle catalyst can be promoted by exploiting metal−support interaction between Pt nanoparticles and molybdenum carbide support. X-ray absorption near edge structure and X-ray photoelectron spectroscopy analyses revealed that Pt atoms exist in more reduced oxidation states in Pt/MMC than those in commercial Pt/C catalysts (Pt nanoparticles dispersed on carbon black). Compared to carbon black support, MMC could donate more electrons to nearby Pt atoms, elevating d-band center of Pt. Electrochemical measurements demonstrated that mass activity and specific activity of the Pt/MMC are 1.6- and 1.5-fold higher than those of commercial Pt/C with the same Pt loading, respectively. This result suggested that the adsorption/desorption strength of reactants (i.e. hydrogen) and reaction intermediates (i.e. hydroxide) was adjusted to the optimized level for efficient HER in alkaline media.

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Synthesis and Characterization of Isomer-Free Quinoidal Small Molecules via Introducing Short Side Chains

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Conjugated molecules based on quinoidal unit have been extensively studied as organic semiconductors for application in OFETs due to its high structural planarity and electron rich characteristics. Their planar structures induce favorable delocalization π-electrons along the conjugated molecules and short π-π stacking distance. Therefore, some of them manifested very promising charge transport characteristics. Recently, quinoidal conjugated molecules containing the isatin terminal unit have been reported because of easy and facile synthesis for forming the quinoidal structure and possibility of introduction into the conjugated polymer backbone. However, isatin terminated quinoidal molecules have the possibility to exist geometrical isomers owing to be connected to double bond between aromatic ring. Thereby, these quinoidal molecules have suffered from purification of unavoidably produced isomers as well as understanding the exact molecular packing model. To obtain the isomer-free isatin terminated quinoidal molecules, we utilized steric effect by incorporating short alkyl and alkoxy side chain into the quinoidal core unit. In this research, we report two quinoidal small molecules, quinoidal methoxy bithiophene (QuMeOBT) and quinoidal ethyl bithiophene (QuC2BT). Furthermore, their thermal, optical, electrical properties, and charge transport behaviors are characterized and discussed.

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Li_3VO_4/Carbon Composite with Enhanced Electrochemical Performances as an Anode Material for Lithium–Ion Batteries

제우진 박한솔 김종식*

동아대학교 화학과

In recent years, lithium-ion batteries (LIBs) have been attractive as energy storage devices because of the development of eco-friendly energy, electric transportation, and electronic devices. LIBs have many advantages such as high power density, low environmental impact, and long cycle life. Despite these advantages, graphite, which is commercially used as an anode material in LIBs, has drawbacks of its low theoretical capacity (374 mAh g^{-1}) and poor stability in charge/discharge processes. Recently, lithium vanadium oxide (Li_3VO_4) has become attractive as an alternative anode material for the LIBs because Li_3VO_4 has a high theoretical capacity (394 mAh g^{-1} at 0.0-3.0 V), fast ionic conductivity, and the lower working voltage range than those of the other metal oxide anode materials. However, Li_3VO_4 suffers from poor electronic conductivity, large band gap, and low Coulombic efficiency, which cause poor the undesirable reversible capacity and rate performance. In this study, we synthesized Li_3VO_4/VGCF composites by using highly conductive vapor grown carbon fiber (VGCF) to overcome the drawbacks of Li_3VO_4. Li_3VO_4/VGCF composites exhibited enhanced electrochemical performance with the reversible capacity of about 310 mAh g^{-1} after 100 cycle at a rate of 0.5 C in the voltage range of 0.0-3.0 V compared to bare Li_3VO_4(about 180 mAh g^{-1}).

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Metal nanoparticle-nanodiamond hybrid nanocatalysts for electrochemical reduction of CO2

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Reduction of CO2 has been receiving increasingly considerable interest in terms of environmental and long term energy-security. An essential requirement for CO2 reduction is to energy-driven flow of electrons with multiple-electron chemical processes that can make C–H and C–C bonds and can cleave C–O bonds. Such processes require a highly efficient catalyst, among which novel metal nanostructures have been regarded as a potential candidate. Here, Au, Ag, and Cu nanoparticles embedded on nitrogen-doped graphitized nanodiamonds (ND) were synthesized as efficient electrocatalysts for the CO2 reduction reaction. The NDs were transformed into the graphitized onion-like form by laser-induced reaction in ethanol, were doped with the N atoms by the thermal annealing under NH3 gas. The metal nanoparticles were directly grown on the graphitized N-doped NDs. We proposed that the efficient performance of these hybrid nanostructures is credited to a synergic effect of the active metal nanoparticles and the pyrrolic-like N electronic structures of NDs. This finding may lead to a new strategy developing cost-effective electrocatalysts for reducing CO2 and converting it into useful chemicals.

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장소: 일산 KINTEX
발표코드: **MAT.P-373**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High-Performance Electrocatalytic Oxygen Evolution of NiFeZn Layered Double Hydroxide

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Highly active and low-cost electrocatalysts for water oxidation are required due to the urgent demands on sustainable solar fuels. However, developing highly efficient catalysts to meet industrial requirements remains a challenge. Layered double hydroxides (LDHs) are a class of layered materials, in which the positively charged layers contain alternately arranged metal cations (they are commonly divalent and trivalent, although monovalent metal cations are also known) balanced by charge-compensating anions positioned within the interlayer space. Due to the rapid development of electrocatalysts, the study of LDHs for oxygen evolution reaction has attracted much attention. Herein, we report a nickel–iron-zinc-layered double hydroxide that shows a current density of 10 mA cm-2 at an overpotential of 350 mV. Such performance is comparable to those of the best-performing nickel–iron-layered double hydroxides for water oxidation. The nickel–iron-zinc-layered double hydroxides can provide high catalytic activity, mainly due to the enhanced conductivity, facile electron transfer and abundant active sites. Our works may expand the scope of cost-effective electrocatalysts for water splitting.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT.P-374**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of metal-MoC hybrid nanospheres for high-performance electrocatalyst

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Vast and exceeding emissions derived from human activities related to fossil fuels have led to an excessive concentration of carbon dioxide (CO2) in the atmosphere with concomitant problems in the environment. To mitigate the resulting harmful effects, CO2 conversion to valuable fuels and precursors have become an urgent need. Recently the design of new cost-effective catalysts able to produce CO and CH3OH from CO2 is a chief challenge. In the current search for new catalysts, transition-metal carbides are appealing as an alternative to novel metals for many reactions due to their abundance, relatively low cost, and, apparently, smaller activation energy barriers for reactions such as for O−O bond cleavage. In the present work, we developed a general and straightforward strategy for the synthesis of molybdenum carbide (MoC) nanospheres by laser ablation of metal oxide in acetone. Crucially, this approach is green, facile, catalyst-free, and especially can be operated under ambient environments. Furthermore, we synthesized metal-MoC hybrid nanostructures that are theoretically predicted to be high activity, selectivity, and stability for the reduction of CO2 to CO with some subsequent selective hydrogenation toward methanol. This green catalytic transformations are very attractive, and promising to overcome low conversion percentages and selectivity reduction of CO2.

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장소: 일산 KINTEX
발표코드: **MAT.P-375**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Cobalt vanadate for efficient electrochemical water oxidation

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Development of high-performance catalysts is very crucial for the commercialization of sustainable energy conversion technologies. Searching for stable, highly active, and earth-abundant multifunctional catalysts has become a critical issue. In this study, we report the synthesis of cobalt vanadate (Co3V2O8) nanosheets and their highly efficient bifunctional electrocatalytic activities toward oxygen evolution (OER) and reduction (ORR) reactions. We observed that Ni-doped Co3V2O8 exhibits excellent catalytic activity and stability for OER and ORR, which is better than Co3V2O8. On the basis of the promising bifunctional activity of the as-obtained catalyst, this electrocatalyst was further integrated into a rechargeable Zn-air battery. This work might provide a strategy to design robust and earth-abundant electrocatalysts for water splitting, and inspire the development of next-generation electrocatalysts for renewable energy applications.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Two-Dimensional Structure of Germanium Arsenide

차승환 박정희[1,*] 차은희[2,*]

호서대학교 그린에너지공학과 [1]고려대학교 소재화학과 [2]호서대학교 제약공학과

The recent discovery of graphene has given rise to significant interest in searching for new two-dimensional (2D) materials with their three-dimensional prototypes, where the 2D layers are stacked with weak van der Waals interactions. One of remarkable properties of the 2D nanostructures is their unique quantum confinement effect at the 2D limit. In the present work, we synthesized the germanium arsenide nanosheets using the exfoliation of bulk crystals that were synthesized by Bridgeman melt-growth method. Bulk GeAs is found to have a band gap (Eg) of ~1 eV, while the GeAs monolayer has been predicted to have Eg = 2.1 eV. We fabricated the Si/GeAs core/shell nanowire array that acts as a photoelectrode in the solar-driven water-splitting reaction, and observed the higher photocurrent with decreasing the layer thickness. First-principles calculations predicted the band alignment between Si and GeAs, and the higher photocurrent for the GeAs monolayers relative to that of the bulk.

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Sulfur doped MoC nanospheres as highly stable electrocatalyst for hydrogen evolution reaction

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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 S-MoC nanocrystals and their excellent electrocatalytic activity. We achieved this by a pulsed laser induced liquid–solid interfacial reaction. S-MoC nanocrystals exhibit excellent HER activity, which demonstrates the best integrated electrocatalytic performance. Finally, This study successfully demonstrates that introducing strain to S-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.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis CoSe2 and NiSe2 for Photoelectrochemical Water Spilliting

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호서대학교 그린에너지공학과 [1]고려대학교 소재화학과 [2]호서대학교 제약공학과

Water splitting is currently an important research topic as it can utilize both water and solar (or electric) energy for a cleaner, recyclable, and cheaper approach to hydrogen generation. Si has long been considered a good candidate material for solar water-splitting photoelectrodes to produce H_2 or O_2. Remarkable progress has been made in recent years toward Si nanostructures that can improve the light absorption capability and increase electrode/electrolyte interfacial charge carrier collection. Moreover, research efforts have also been devoted to combining Si with earth-abundant catalysts for H_2 and O_2 evolution and reduction (HER and OER). In the present work, we developed $CoSe_2$ and $NiSe_2$ coupled with a Si nanowire array that acts as a promising bifunctional photoelectrode in the solar-driven water-splitting reaction. .

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장소: 일산 KINTEX
발표코드: **MAT.P-379**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Enhancing intrinsic stability of CsPbI3 nanowires by introducing Bromide

서재민 박정희[*] 박기동[1,*] 김준동[2,*]

고려대학교 소재화학과 [1]고려대학교 미세소자공학협동/마이크로소자 [2]고려대학교 신소재화학과

Cesium lead tri-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 chemical vapor deposition (CVD) growth of CsPbI3 nanowires that maintain black cubic phase at room temperature. Nevertheless, the resulting cubic phase CsPbI3 nanowires turn 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.

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Synthesis of two composition of zinc phosphide for photodetector

이준영 박정희[1,*]

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Semiconductor alloy nanowires (NWs) have recently attracted substantial attention for applications in optoelectronic nanodevices because of many remarkable properties, including band gap tunability. Both zinc and phosphorus are found abundantly in the earth’s crust, and also both are nontoxic, which is the appropriate material for manufacturing semiconductor alloy NWs. Herein, we synthesized phase-tuned zinc phosphide composition, Zn3P2 NWs and ZnP2 NWs with different crystal structures by controlling the growth conditions during chemical vapor deposition. The first type of synthesized NWs, Zn3P2, was tetragonal crystal structure and grew uniformly along the [110] direction. And the second, ZnP2 NWs, was monoclinic crystal structure and grew uniformly along the [100] direction. The change in the crystal phase triggers a result of the increase of the P element during growth. The changes of electrical and optical properties were studied through the band-gap energy identification using UV-vis spectroscopy and the phase change according to the ratio of Zn and P in the NWs through the electrodes fabricated by the lithography process.

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All Inorganic Perovskite Nanowire Lasers

박기동 김준동[1] 정성현[2] 서재민[3] 이진하[4] 박정희[3,*]

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Light−matter interactions in inorganic perovskite nanolasers are investigated using single-crystalline cesium lead halide ($CsPbX_3$, X = Cl, Br, and I) nanowires synthesized by the chemical vapor transport method. The perovskite nanowires exhibit a uniform growth direction, smooth surfaces, straight end facets, and homogeneous composition distributions. Lasing occurs in the perovskite nanowires at low thresholds (3 μJ/cm^2) with high quality factors (Q = 1200−1400) under ambient atmospheric environments. The wavelengths of the nanowire lasers are tunable by controlling the stoichiometry of the halide, allowing the lasing of the inorganic perovskite nanowires from blue to red. The unusual spacing of the Fabry−Pérot modes suggests strong light−matter interactions in the reduced mode volume of the nanowires.

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발표분야: 재료화학
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Synthesis of Two-Dimensional Gallium Chalcogenide(S,Se) monolayer via Controlled Chemical Vapor Deposition

김도연 박기동[1,*] 김준동[2,*] 박정희[*]

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Recently, Many groups pay attention to 2D materials and their fascinating properties.we are successfully synthesization one kind of post transition metal-mono chalcongenide monolayer(GaS,GaSe). Gallium sulfide and Gallium selenide is a typical layered metal –mono chalcongenide, which consist of hexagonal phase.Before our group reported the HSE06 calculation identified an indirect band gap for the GaS and GaSe monolayers of 3.325 and 3.001 eV, respectivley.And now we can additionally S and Se of GaSxSe1-x composition tuning. Herein, we synthesized GaSe, GaS and GaSSe monolayer via chemical vapor deposition method. The size, shape, and thickness of the GaSe, GaS and GaSSe monolayer were controllable by growth duration, growth temperature, and gas flow rate. Large-area and single-crystalline GaSe, GaS and GaSSe monolayers were successfully synthesized with a thickness of 0.8 nm and a width of 10~20 µm.

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Composition Tuned $(GaAs)_{1-x}(Ga_2Se_3)_x$ Ternary Alloy Nanowires

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Multicomponent nanowires (NWs) are of great interest for integrated nanoscale optoelectronic devices owing to their widely tunable band gaps. In this study, we synthesize a series of $(GaAs)_{1-x}(Ga_2Se_3)_x$ 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 = 0-0.5 allowed the tuning of the band gap (1.4–2.0 eV). Pure GaAs NWs were synthesized with [111] growth direction using a hydrogen gas flow during the growth. As the Ga_2Se_3 incorporated during the growth under H_2 flow, the NW becomes defect-free single-crystalline and their growth direction is converted homogeneously into [110]. The Ga vacancies of Ga_2Se_3 along the [110] direction may also contribute to produce the uniform growth direction of NW. The incorporation of Se into the GaAs nanowires induces higher photo-sensitivity and lower dark current, which opens up a new strategy for enhancing the performance of photodetectors

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Eco-friendly preparation and mechanical behaviors of graphene oxide/carbon nanotube-filled sodium carboxymethyl cellulose nanocomposites

손영래 박수진*

인하대학교 화학과

Sodium carboxymethyl cellulose/graphene oxide/carbon nanotubes (CMC/GO/CNT) nanocomposites were prepared by a simple solution mixing-evaporation method as a function of CNTs amount. As GO/CNT complexes are formed, CNTs can be dispersed in water, indicating that the GO/CNT-filled CMC nanocomposites are prepared environmentally friendly. X-ray diffraction (XRD) and scanning electron microscope (SEM) were used to investigate the structural properties and morphologies, respectively. The mechanical properties of CMC/GO/CNTs nanocomposite films were analyzed by universal testing machine (UTM). Compared with pure CMC film and CMC/GO nanocomposite film, it was found that the mechanical properties of CMC/GO/CNTs nanocomposite films were enhanced with adding the CNTs.

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Preparation of micro-capsules containing phase change materials for high efficient thermal energy storage

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In this study, the manufacturing process of micro-capsulated phase changing materials (PCM) for thermal storage performance of latent heat was investigated. The paraffin/expanded graphite (EG)/melamine-type resin micro-capsulated PCM were prepared with different ratio of EG. The paraffin wax was used as inner materials and the melamine-type resin was used as micro-capsule materials for thermal energy storage system. EG was also used as an additive for thermal conductivity. The surface and structural properties of the PCM were determined by scanning electron microscopy (SEM) and X-ray diffraction (XRD), respectively. The thermal energy storage and thermal properties of the PCM were studied by differential scanning calorimetry (DSC), thermal conductivity (TC), and thermogravimetric analyzer (TGA).

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Characterization of poly(vinyl alcohol) hybrid films containing graphene oxide for gas barrier

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Recently, polymeric gas barrier films have been successfully contending over traditional materials (glass, wood, metal, and ceramic) in the field of food packaging, liquid crystal displays, hydrogen storage, pharmaceuticals, and flexible electronics. In this work, we prepared the gas barrier hybrid films using the graphene oxide (GO)/poly(vinyl alcohol) (PVA) composites. The morphology and structure of the hybrid films were confirmed using the transmission electrical microscope (TEM) and X-ray diffraction (XRD), respectively. The oxygen permeability rate (PO2) of the hybrid films was measured with an oxygen permeability tester in accordance with ASTM D-3985 at 23 °C and 0% relative humidity. The transparency of the hybrid films was evaluated using ultraviolet visible spectroscopy.

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Synthesis and Analysis of N-doped TiO_2 and Ceramic-coated TiO_2

유리 김유진*

한국세라믹기술원 엔지니어링세라믹센터

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. A great deal of effort has been devoted to improving efficiency of with the pigments such as using chlorine method. To retain and enhance the whiteness and reflectivity of white pigment, we adopted core-shell system. Also, nitrogen doped titanium dioxide(N-doped TiO_2) is attracting a continuously increasing attention because of its potential as material for environmental photo-catalysis. The N-atoms can occupy both interstitial and substitutional positions in the solid, with some evidence for a preference for interstitial sites. N-doped TiO_2 powders were obtained by sol–gel synthesis. Also, 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 N-doped TiO_2 and ceramic-coated TiO_2 samples were characterized by UV-vis, CIE Lab color parameter measurements, TEM (transmission electron microscopy) and XRD (powder X-ray diffraction)

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Hierarchical Magnetic Nanoparticles for Heavy Metal Removal

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Hierarchical magnetic nanoparticle, IO@PD@MNP was synthesized by a successive coating of polydopamine and iron oxide nanoneedles onto magnetic core. The structure of the IO@PD@MNP was characterized using scanning electron microscopy, transmission electron microscopy and X-ray diffractometer. The IO@PD@MNP exhibited excellent removal efficiency for heavy metal ions such as Pd(II), and Cr(VI) showing that 10 ppm of heavy metal ions was completely removed within 20 min. Excellent magnetic property of IO@PD@MNP made it simple to recover from the solution by an external magnetic field and to be effectively reused. The removal efficiency effects on the thickness of polydopamine layer and the pHs will be further studied.

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Bimetallic PdNi nanoparticles supported on the carbon nanotubes for efficient catalysis for nitrophenol reduction

김지당 최현철*

전남대학교 화학과

Carbon nanotubes (CNTs) make as an ideal candidate for supporting material due to their outstanding physical properties, such as the ultra-high surface area, high mechanical strength, and also high chemical and thermal stability. Recently, many metals (Pt, Au, Pd, Ag, Ru, and Ni) have been successfully deposited onto the surface of CNTs for obtain the carbon based on metal nanocomposites, and which showed remarkable advantage in improving catalytic efficiency. Aromatic nitro compounds are the pollutants in wastewater. Pd-based compounds have high catalytic activity for the reduction of aromatic nitro compounds. By the way, the applications of Pd nanoparticles remain limited by weakness in terms of their easy aggregation and the difficulty of catalyst product separation. In this study, we synthesized Pd and Ni-decorated CNT by introducing thiol groups on CNTs. The thiol of surface modification is an effective way to obtain dispersed Pd and Ni nanoparticles on the surface of CNT. To study the catalytic activity, a 1 x 10-3 M of aqueous nitrophenol solution was mixed with 0.1 M of fresh NaBH4 solution. The Pd/Ni-CNT catalysts were added and stirred. The mixture was immediately transferred into a quartz cuvette and UV-vis absorption spectra were recorded to monitor changes in the reaction mixture. The samples were characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and transmission electron microscopy (TEM). The reduction kinetics of aromatic nitro compounds is also investigated by ultraviolet-visible (UV-vis) measurement.

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Effective removal of heavy metal ions and organic dyes with core-shell structured carbon@iron oxide nanoneedles

진예진 이하진[1,*]

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Core-shell structured iron oxide nanoneedles (IO-NNs) with or without organic polymer core were synthesized by a temperature-controlled heat treatment of iron oxide nanoneedles grown on spherical polymer template. The structure of the IO-NNs was characterized by scanning electron microscopy, X-ray diffractometer, FT-IR, and thermal gravimetric analyses. Due to a synergistic effect of IO nanoneedles and organic core, the IO-NNs with organic polymer core (IO-oNNs) showed a good removal efficiency for heavy metal ions, Pb(II) and Cu(II) showing adsorption capacities of 123.4 mg/g and 32.7 mg/g, respectively. In addition, the IO-oNNs exhibited an excellent photocatalytic activity in the degradation of methylene blue (MB) and methyl orange (MO) visible light irradiation, which showed the degradation efficiency of 99.7% and 99.5% for the MB and MO degradation within 20 minutes. The further systematic studies on the inorganic and organic pollutant removal by the IO-NNs, such as effects on the pH of the solvent, concentration of pollutants, and dosage of the IO-NNs will be presented in detail.

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Flowerlike layered double oxide (LDO) nanocrystals with ultrafast removal efficiency for heavy metal ions and toxic organic pollutants

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Heavy metal ions existing in natural underground water and drinking water are causing environmental issues and global health concerns. Especially, arsenic [As(V)] and chromium [Cr(VI)] are hazardous pollutants, that causes serious risks to human health, living organisms and the ecological system. Herein, flowerlike Mg/Fe layered double hydroxide (MF-LDH) nanocrystals were prepared by a simple hydrothermal method for removal of As(V) and Cr(VI) from contaminated water. After the thermal treatment of MF-LDH nanocrystals at 400 oC, the MF-LDH was converted into their corresponding oxide, Mg/Fe layered double oxide (MF-LDO), which also maintained the flowerlike structure. The crystal structure, morphology, microstructure and chemical structure were characterized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy; energy dispersive X-ray spectroscopy mapping, X-ray photoelectron spectroscopy, and Fourier transform infrared spectroscopy. The MF-LDO nanocrystals showed superb removal efficiency for both As(V) and Cr(VI), which showing over 97% removal within 5 min and providing maximum removal capacities of 178.5 mg/g [As(VI)] and 129.7 mg/g [Cr(VI)]. In addition, Au nanoparticles were successfully introduced in the MF-LDO nanocrystals and the products exhibited excellent catalytic conversion rate for reduction of 4-nitrophenol into 4-aminophenol (100% conversion in 5 min). This work provides simple, convenient and cost effective strategies to develop promising materials for water pollutant removal.

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Comparing glycerol binding on PtRu surfaces for understanding glycerol electrooxidation reactions

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한국화학연구원 화학시뮬레이션센터 [1]한국화학연구원 탄소자원화연구소

Converting glycerol into high-value chemicals becomes important as large amount of glycerol is obtained as a byproduct of manufacturing biodiesel, an alternative to fossil fuels. Recently, several groups have reported glycerol conversion techniques on the basis of electrochemical processes. For example, glycerol molecules are electrochemically oxidized on PtRu-alloy surfaces with an enhanced catalytic activities compared to the pure Pt surface. In this poster, we will compare binding energies of glycerol molecules on Pt and PtRu-alloy surfaces with computational investigations. As expected, glycerol molecules strongly bind to positively charged Ru sites in the surface. To understand different catalytic activities of Pt and PtRu-alloy surfaces, we also discuss our findings with experimental observations.

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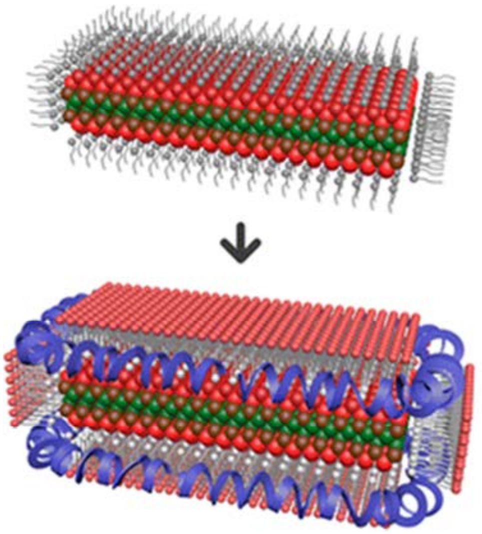
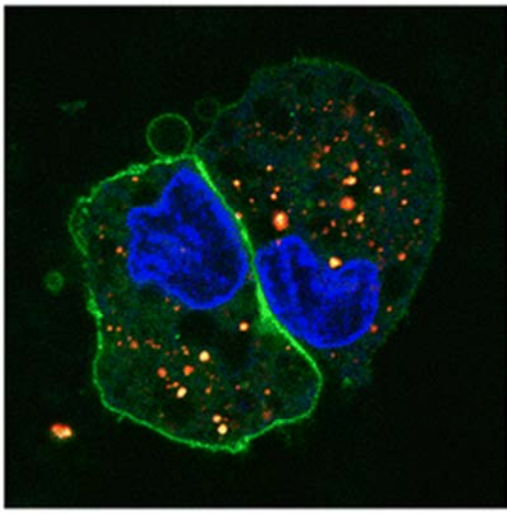
Lipoprotein Nanoplatelets: 2D Fluorescent Nanoprobe with Rapid Cellular Entry

임성준

DGIST 지능형소자융합연구실

Semiconductor nanoplatelets (NPLs) are 2D fluorescent nanocrystals that have recently attracted considerable attention due to their quantum-well-like physics, atomically precise thickness, and unique photophysical properties such as narrow-band fluorescence emission. Here we introduce a new colloidal nanomaterial that is a NPL coated with phospholipids and lipoproteins. The phospholipids adsorb to flat surfaces on the NPL, and lipoproteins bind to sharp edges to enable monodisperse NPL encapsulation with long-term stability in biological buffers and high-salt solutions. The lipoprotein NPLs (L-NPLs) are highly fluorescent, with brightness comparable to that of wavelength-matched quantum dots at both the ensemble and single-molecule levels. They also exhibit a unique feature of rapid internalization into living cells, after which they retain their fluorescence. These unique properties suggest that L-NPLs are particularly well suited for applications in live-cell single-molecule imaging and multiplexed cellular labeling.Reference: Lim et al., J. Am. Chem. Soc. 2016, 138, 64-67.





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발표종류: 포스터, 발표일시: 금 13:00~14:30

Development and characterization of molybdophosphoric acid captured polyether ether ketone composite membrane for water electrolysis

김민진 김보영 정장훈[1,*]

명지대학교 화학과 [1]명지대학교 자연과학대학/화학과

Molybdophosphoric acid (MoPA) captured polyether ether ketone (PEEK) composite membrane for water electrolysis has been investigated. The composited membrane, covalently cross linked (CL) sulfonated polyether ether ketone (SPEEK) with a captured MoPA, was prepared in sulfonation of PEEK, cross linkage reaction with 1,4-diiodobutane, and addition with MoPA. PEEK was covalently cross-linked with 1,4-diiodobutane to improve mechanical strength and was added MoPA to increase proton conductivity. MoPA should be fixed to back bone of SPEEK to prevant bleeding out. Therefore, the carbonyl group of SPEEK was reduced with $NaBH_4$ and 3-isocyanatepropyltriethoxysilane (ICPTES) was added. The MoPA captured composite was produced was produced in reaction MoPA with 3-mercaptopropyltrimethoxysilane (MPTMS). In conclusion, MoPA with CL-SPEEK composite membrane featured 0.0987S/cm of proton conductivity at 80℃, and 2156 hours of chemical stability in Fenton test. These properties are better than those of membrandes of other SPEEK system.

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Laser Induced Patterning of Co-Ni alloy/Reduced Graphene Oxide Hybrids Composites on Graphene Oxide Film and its Application

이상화 이민형*

경희대학교 응용화학과

Due to the miniaturization and portability of electronic devices, the development of simple manufacturing methods for electrodes with complex pattern and small sizes has received much attention due to public interest in flexible micro-scale electronic devices. Electrochemical capacitor or supercapacitor has been attracted by high volumetric energy density, power density and fast charge-discharge rate and homogeneous distribution transition metal nano-particles with rGO can help to enhance chemical, electrical coupling effects with high electrical conductivity. Synthesis of layered double hydroxide(LDH)/GO composites film is solution of one-pot patterning of transition metal/graphene composites which can improve energy density and power density of MSC and activate oxygen evolution reaction(OER) performance. Here, Co-Ni/rGO composites has been selectively grown by laser induced photothermal reactions of graphene oxide film on flexible substrate. Patterned Co-Ni/rGO electrodes show excellent electric conductivity compared to bare rGO, and this advantage could be contribute to increase power density. In addition, Co-Ni/rGO can be used for OER application as well as energy storage capability.

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Flexible Piezoelectric Nanogenerators Using Fe-Doped BaTiO3 Sol-Gel Pillars

최성영 이민형[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

Piezoelectric generators, harvesting energy from mechanical stimuli in living life, are attractive for many applications. BaTiO3 is one of the promising materials suitable for piezoelectric generators because it is lead-free and has high piezoelectric coefficient. In this study, hexagonal arrays of Fe-doped BaTiO3 sol-gel were easily fabricated on flexible ITO/PET film using PDMS stamps and Its dipoles were aligned through the poling process. The repetitive pillar arrays enhanced the effect of dipoles resulting in increasment of output voltage and current of up to 10 V and 1 uA. The iron ions were used as dopant for improving the low conductivity of BaTiO3.

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Synthesis and Characterization of Cu doped TiO2 hollow spheres with enhanced optical absorption and photocatalytic activity

장수관 배재영*

계명대학교 화학과

In this study, Cu-doped TiO2 hollow spheres with different doping contents from 0 to 6.0 wt% were synthesized via sol−gel method to shift the absorption threshold to the visible light region. The resulting materials were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), Brunauer-Emmett-Teller method (BET) analysis and ultraviolet-diffuse reflection spectroscopy (UV-DRS). TEM images show that the size of Cu-doped TiO2 hollow spheres were about 200-300 nm. The main peaks observed in the XRD pattern clearly reflect the monoclinic phase of the nanomaterials and BET surface area was confirmed to be 50-60 m2/g. UV–DRS shows that the nanomaterials were absorbed in the range of 200–800 nm, supporting that it can be used in visible spectrum of light. The photocatalytic activity of nanomaterials was confirmed by degrading 15 mg/L methylene blue under the visible light irradiation.

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All-in-one inkjet printing for paper-based thermoelectric sensor, heater and digital microfluidic chip

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서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

Recently the paper electronics has attracted a huge attention due to its powerful advantages of simple CAD design, easy printing and drawing fabrications, and affordable manipulation. Among the merits, printing is a critical factor in the developing field of the printing paper electronics. Various functional ink materials, such as silver nanoparticle (AgNP), PEDOT:PSS and carbon nanotube (CNT), for inkjet printing on paper substrate have been formulated and investigated, in order to fabricate the paper-based temperature sensor and heater and then to integrate on a paper-based electromicrofluidic lab-on-a-chip, referred to active microfluidic paper chip. Utilizing the thermoelectric effect of p-type PEDOT:PSS with the junction of metal AgNP by inkjet printing, the linear responses of Seebeck coefficient, 8.681 V/K was achieved, indicating the positive possibility for usage of the temperature sensor in film type. Micro heater printed on paper with AgNP ink showed the uniform thermal distribution, which was analyzed by using the infrared imaging camera (FLIR) and the PEDOT:PSS-based paper temperature sensor. These two elements were integrated on an active microfluidic paper chip, which was also fabricated by using printing conductive material ink. For future work, the performance of thermal fluidic manipulations will be investigated to achieve the final goal the complete integration of printing- and paper-based active microfluidic chip, to be used for the endothermic chemical reactor just on the paper.

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Catalytic reduction of CO_2 to hydrocarbon via ferroelectric material $PbTiO_3$ poling

고아라 이민형*

경희대학교 응용화학과

CO_2 was regarded as the main culprit of the global warming. But now it can be considered a carbon source. Consequently, catalytic conversion of CO_2 into fuels or other hydrocarbon materials has draw attention. It has many pathway to convert CO_2 into other materials. Each products of the conversion has different standard reduction potential. So, if we can tune the band position, it can be possible to enhance the selectivity of the reaction. In this work, among the many catalytic materials, we concentrate on the oxide ferroelectric material $PbTiO_3$(PTO). The different condition of polarization in PTO has different degree of band bending. So when we change the polarization condition by external field, we can control the main product of the CO_2 conversion.

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장소: 일산 KINTEX
발표코드: **MAT.P-400**
발표분야: 재료화학
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Fabrication of nanostructured vanadium oxide thin film for smart window applications

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부산대학교 화학공학과 [1]부산대학교 화공생명공학부

Vanadium oxide represents an important class of thermo- and electrochromic materials employed in different technological applications such as intelligent window coating materials, catalyst, cathodes in Li-ion batteries, or in electrical, optical, temperature sensing or switching devices. 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.Here, 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.

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발표분야: 재료화학
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FeOF Nanoparticles Anchored on Reduced Graphene Oxide (r-GO) as a Cathode Material for Lithium-Ion and Sodium-Ion Batteries

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동아대학교 화학과

Iron oxyfluoride (FeOF) is one of the most promising cathode materials for lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs) because of its low cost, non-toxic, and high theoretical capacities (about 590 mAh g^{-1} at 1.5-4.0 V and 885 mAh g^{-1} at 1.2-4.0 V, respectively in LIBs, and about 788 mAh g^{-1} at 1.0-4.0 V in SIBs), compared with previous reported cathode materials such as $LiFePO_4$ (170 mAh g^{-1}) and Na_2FePO_4 (154 mAh g^{-1}). However, FeOF shows poor cycling stability and rate capability due to its low electronic conductivity and ion diffusion coefficient. In this work, the FeOF/reduced graphene oxide (r-GO) nanocomposites with about 10 and 20 wt% of the r-GO contents were synthesized through solvent-thermal treatment of $FeSiF_6 \cdot 6H_2O$ in 1-propanol solution. FeOF/r-GO samples showed the improved initial discharge capacities of about 314 mAh g^{-1} at 1.5-4.0 V and about 380 mAh g^{-1} at 1.2-4.0 V with a current density of 50 mA g^{-1}, respectively, compared to bulk FeOF in LIBs. The FeOF/r-GO nanocomposites also exhibited superior cycling stabilities to bulk FeOF at 1.0-4.0 V and a current density of 20 mA g^{-1} in SIBs.

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장소: 일산 KINTEX
발표코드: **MAT.P-402**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Bismuth Iron Oxide(BFO) Perovskite as Catalyst for efficient CO_2 reduction via poling process

황예윤 이민형*

경희대학교 응용화학과

The carbon capture and utilization(CCU) technology for reducing CO_2emissions is a technology attracting attention as it can reduce CO_2concentration in the atmosphere as well as convert CO_2 into high value-added carbon sources. In addition, since the thermodynamic reduction level of CO_2 is very dense, development of a catalyst is very important for selectively producing various carbon sources. In our experiment, Bismuth Iron Oxide (BFO) was used as a catalyst for CO_2 reduction. To obtain high purity BFO, we use an inexpensive and simple synthesis method using glycine and annealing by CVD.BFO has high-temperature ferroelectric and piezoelectric properties. In this study, we focused on these dipole-induced poling characteristics (ferroelectric polarization)of BFO. Therefore, various carbon sources at the CO_2 reduction potential can be obtained and the product can be confirmed by Gas Chromatography (GC),

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Au-Cu_2O Heteronanocrystals with Intended Configurations for Plasonic Photocatalysis

위대한 홍종욱[1] 한상우[*]

KAIST 화학과 [1]울산대학교 화학

Precise control over the topology of plasmonic metal-semiconductor heteronanostructures is essential for fully harnessing their plasmonic function and hence for designing innovative solar energy conversion platforms. Here, we present a rational synthesis strategy for the realization of plasmonic metal-semiconductor heteronanocrystals with intended configurations through the site-selective overgrowth of semiconductor Cu_2O on desired sites of anisotropic Au nanocrystals. Both the exploitation of structural characteristics of Au nanocrystals and the selective stabilization of their surfaces are keys to the construction of heteronanocrystals with a specific configuration. Our approach can provide an opportunity to precisely explore the link between the solar energy conversion efficiency and the structure of heteronanocrystals as well as to obtain important insights into the underpinning mechanism. Heteronanocrystals produced by Cu_2O overgrowth preferentially on the multiple high-curvature sites of Au nanocrystals exhibited prominent photocatalytic hydrogen production activity due to efficient charge separation by strong plasmon excitation at the Au- Cu_2O interface and subsequent sustainable hot electron transfer from Au to Cu_2O.

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PVA-assisted combustion synthesis and CO_2 absorption properties of KNO_3-K_2CO_3-MgO absorbent at intermediate temperature

<u>오경렬</u> 곽진수 김강영 ATILA GULBAHAR 권영욱*

성균관대학교 화학과

CO_2 is the main source of greenhouse gas problem. Among various techniques, carbon capture and storage (CCS) is the most promising solution for the mitigation of global warming. The study of CO_2 capture at intermediate temperature (200-500℃) is performed mainly by alkali metal nitrate and carbonate promoted MgO absorbents. In this study, KNO_3–K_2CO_3 promoted MgO absorbent was synthesized by combustion method and its structure and CO_2 capture properties were analyzed by XRD, IR and TG. Polyvinyl alcohol (PVA) was used as a complexing agent for metal cations and as a fuel for combustion process. KNO_3 was used as an oxidizer for the combustion of PVA and partially converted into K_2CO_3 which is necessary for fast CO_2 absorption kinetics. The degree of conversion from KNO_3 to K_2CO_3 was dependent on the amount of PVA used. Temperature swing CO_2 absorption (TSA) and isothermal CO_2 absorption test shows that this absorbent has several reaction steps as temperature increases or time goes by. The CO_2 absorption properties of the absorbent were further measured by cycle test.

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Interconnected Silicon Nanoparticles through Ultrathin Cellulose Nanofibers Derived Carbon for High Performance Lithium Ion Battery Anode

김종민 오지섭 박원철*

서울대학교 융합과학기술대학원 융합과학부

Silicon has high theoretical capacity, ~ 4200 mAh g^{-1}, and it is naturally abundant, which makes it a good alternative for conventional graphite anode material. However, its bad cycling stability owing to a volume expansion/contraction during cycling and low intrinsic electric conductivity blocks the way to practical use. We developed interconnected silicon nanoparticles through ultrathin cellulose nanofibers derived carbon. It shows 72.2 % (808 mAh g^{-1}) of capacity retention after 500 cycles and 464 mAh g^{-1} at 8 A g^{-1}. On the other hand, bare silicon nanoparticles exhibit only 19.7 % (253 mAh g^{-1}) of capacity retention and 178 mAh g^{-1} at the same condition. Silicon nanoparticles are mixed with TEMPO-oxidized cellulose nanofibers and then freeze-dried to form a brown aerogel. After pyrolysis, cellulose nanofibers carbonize into graphitic carbon. Ultrathin cellulose nanofiber derived carbon entangles each silicon nanoparticle to form a micro-sized chunk. This micro-scale interconnection between silicon nanoparticles through carbon network can provides high electric contact area as well as a volume expansion suppression for silicon nanoparticles. Moreover, the carboxylic group of ultrathin cellulose nanofibers (thickness of 1.55 nm ± 0.532) makes adhesive to the native oxide layer of silicon via hydrogen bonding/covalent bonding. At high thickness, an electrode with CMC or PAA binder is very brittle so unable to be used in a real application. With this structure, no brittle electrodes are observed at high thickness (160 μm). Therefore, this material has a great potential for lithium ion batteries anode.

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The study on wettability of hexagonal boron nitride

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UNIST 에너지공학과 [1]UNIST 화학과

Hexagonal boron nitride (h-BN) films can be used as protective layers of metal due to their extraordinary chemical and thermal stability. The wettability of h-BN plays a key role in adhesion to certain substrate. The origin on the wettability and the effect of hydrocarbon contamination on the wettability of h-BN were recently reported using the measurement of water contact angle.[1] However, the specific surface energy and effects on other gases of h-BN have not been well investigated even though many researchers have studied the structural and electrical properties of h-BN. In this presentation, we will explain the wettability and the surface energy of h-BN calculated by using various calculation methods from the contact angle measurements on h-BN films. The h-BN films were grown on single crystal platinum substrate by the chemical vapor deposition method. The contact angle measurements of the h-BN film were carried out by using polar water and nonpolar diiodomethane. Furthermore, we investigated influence of air contamination on the surface energy of h-BN.References [1] Li. X, Qiu. H, Liu. X, Yin. J and Guo. W, Adv. Funct. Mater., 2016, 10, 1002.

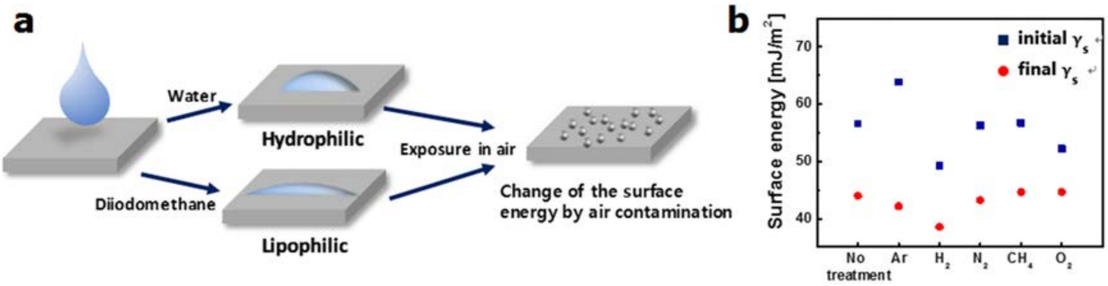

Figure 1. **(a)** Scheme about the overall measurements of contact angle. Water and diiodomethane are used in contact angle measurements. **(b)** The variation of surface energy after gas treatment.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of cobalt metal decorated-nitrogen doped mesoporous graphene composites and their application for electrochemical hydrogen storage

서명덕 이지혜 정 현*

동국대학교 화학과

We successfully synthesized cobalt metal decorated-nitrogen doped mesoporous graphene composites (Co-NMG) through the reaction between $Co_2(CO)_8$ and nitrogen doped mesoporous graphene (NMG). The pristine NMG was synthesized by hydrothermal treatment of graphite oxide (GO), self-assembled triblock copolymer (Pluronic P-123) and ammonium hydroxide. And then, the Co-NMG was obtained by refluxing with the NMG and $Co_2(CO)_8$ as a cobalt precursor in 1,2-dichlorobenzene. To find the optimal weight ratio with the highest hydrogen storage capacity, we controlled the weight ratios of NMG and $Co_2(CO)_8$. The obtained Co-NMGs were characterized by X-ray diffraction (XRD) measurement, field emission scanning electron microscopy (FE-SEM), and energy dispersive spectrometry (EDS). The specific surface area and pore size of obtained samples were investigated by N_2 adsorption-desorption isotherms measurement. Furthermore, hydrogen storage properties of prepared samples measured using cyclic voltammetry and galvanostatic charge-discharge tests in a three-electrode system in KOH.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-408**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Ambipolar Organic Light Emitting Transistors based on Pentacene and Perylene Produced by Neutral Cluster Beam Deposition

이명재 김대규[1] 최종호[1,*]

고려대학교 일반대학원/화학과 [1]고려대학교 화학과

Fabrication of π-conjugated tetracene-based light-emitting transistors first reported in 2003 offered a novel combination of both switching and EL characteristics in single device, leading to a new category of functional devices known as organic light-emitting field-effect transistors (OLEFETs). Heterojunction-based OLEFETs with a top-contact, long channel geometry were fabricated and comparatively characterized. The neutral cluster beam deposition (NCBD) method was used to successively deposit two layers of p-type pentacene and n-type P13. Also, we present the effects of asymmetric electrodes on the device performance of the OLEFETs. On the basis of the growth of high-quality and well-packed crystalline thin films, the OLEFETs show good field effect characteristics, well-balanced ambipolarity, and electroluminescence (EL) under ambient conditions. In comparison with the OLEFETs with symmetric electrodes (Au-Au), the OLEFETs with asymmetric electrodes (Au-LiF/Al) exhibited significantly enhanced EL around both source and drain electrodes under ambient conditions. The significantly improved EL is attributable to better electron carrier injection using the low work function electrodes. The operating EL mechanisms responsible for the observed recombination zone are discussed with the aid of light-emission images obtained using charge-coupled devices (CCD).

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발표코드: **MAT.P-409**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Pd nanodot-modified Au Nanoparticles with Graphene Interface for Efficient Visible-Light Induced C-C Coupling Reaction

강은미 임동권[1,*]

고려대학교 NBIT [1]고려대학교 KU-KIST 융합대학원

The use of plasmonic nanoparticle with Pd nanoparticle enabled to increase the photocatalytic activity of Pd nanoparticle by harvesting the visible region of light and transfer of hot-electron from Au to Pd nanoparticle. In this work, we focused on the effect of interface layer between Au and Pt nanoparticle. To demonstrate this hypothesis, we prepared Pd-nanodot modified AuNPs, Pd-nanodot modified GO-AuNPs and Pd-nanodot modified r-GO AuNPs. The fastest reduction rate of Fe3+ into Fe2+ was observed in case of Pd-rGO-AuNPs because of the fast electron transfer by reduced graphene oxide layer. Also, we performed Suzuki coupling reactions to demonstrate the role of graphene interface 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. Upon plasmon excitation, catalytic reactions occur through both plasmonic photocatalytic and photothermal conversion. Under the illumination of Xe lamp at 5.24 W/cm2, Pd-rGO-AuNP obtained fast reaction rate compared to the case without interface. It showed higher reaction rate compared to the case of same temperature (50 ℃) and no light. The presence of reduced graphene oxide (rGO) layer was critical in obtaining an efficient visible-light induced photocatalytic reaction for C-C coupling.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-410**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and characterization of the carbamoyl phosphine oxide moiety functionalized nitrogen doped mesoporous graphene

김현주 이지혜 정 현*

동국대학교 화학과

Carbamoyl phosphine oxide moiety functionalized nitrogen doped mesoporous graphene (CMPO-NMG) was successfully synthesized by amide coupling reaction with triethyl phosphonoacetate and the pristine nitrogen doped mesoporous graphene (NMG). The pristine NMG was obtained by the pyrolysis of the as-prepared NMG, in which it was synthesized by hydrothermal process of graphite oxide (GO), triblock copolymer (Pluronic P123), and ammonium hydroxide as a nitrogen source, under argon gas flow. The obtained CMPO-NMG was characterized by measurements of powder X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDS) and Fourier transform infrared spectroscopy (FT-IR). The specific surface area and pore structure of CMPO-NMG was also investigated by N_2 adsorption-desorption isotherm measurement.

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장소: 일산 KINTEX
발표코드: **MAT.P-411**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Pd-nanodot Decorated MoS2 micro/nano complex for Highly Efficient Visible-Light Induced Photocatalytic Suzuki-Miyaura Coupling Reaction

신현호 강은미[1] 임동권[2,*]

고려대학교 KU-KIST융합대학원 [1]고려대학교 NBIT [2]고려대학교 KU-KIST 융합대학원

Two dimensional (2D) materials such as molybdenum disulfide (MoS2) have recently attracted scientific attentions because of their various applications in catalysis, energy devices, etc. Here, we report palladium nanodot decorated MoS2 micro/nano sheet as a highly efficient visible-light responsive photocatalyst for Suzuki-Miyaura coupling reaction. The presence of MoS2 increased the reaction rate of the C-C coupling reaction with visible light because of the band gap structures of MOS2 and electron transfer process. In this poster, we are going to provide the detailed experimental parameters and results that performed to unveil the underlying mechanism of the enhanced photocatalytic activity of Pd-2D hybrid nanomaterials.

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발표코드: **MAT.P-412**
발표분야: 재료화학
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Carbon Nanotube-framed Membrane for Skin Heat Signal-Responsive Transdermal Drug Delivery: Dramatic Drug-Loading and Thermally Controlled Drug-Releasing Characteristics

강지혜 신원상[1,*]

단국대학교 나노바이오의과학과 [1]단국대학교 나노바이오의과학

Skin heat signal-responsive CNT membranes were prepared by self-assembling of CNT fibers hybridized with chitosan (Chit) in core-shell structure and then by chemical integration of a temperature-responsive copolymer, poly(NIPAAm-co-BVIm) (or pNIBIm), as an additional outer shell. The membranes with different Chit/CNT ratios and constant pNIBIm concentration, Chit-CNT25-pNIBIm, Chit-CNT50-pNIBIm, Chit-CNT75-pNIBIm, have three dimensionally interwoven porous nanostructure. Scanning electron microscopy clearly showed the temperature-responsive swelling and deswelling characteristic of the triple core-shell structured Chit-CNT-pNIBIm fibers. Temperature-responsive bovine serum albumin (BSA)-loading and -releasing tests were attempted at the various temperatures such as 4℃ (refrigerator temperatures), 25℃ (room temperature), 36 ℃ (body temperature), and 40℃ (>body temperature). Chit-CNT50-pNIBIm hybrid membrane showed dramatically high loading capacity of 9.7 mg per 1 mg membrane at 4℃. The membrane also showed a temperature-dependent BSA-release characteristic, for instance, about 0.39 mg at 25℃, about 0.92 mg at 36℃, and about 3.41 mg at 40℃ per 1 mg membrane. The Chit-CNT-pNIBIm hybrid membranes showing highly effective drug-loading/-releasing characteristics could be potentially used as skin heat signal-responsive transdermal drug delivery system in the medicinal field and tissue regeneration area.

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장소: 일산 KINTEX
발표코드: **MAT.P-413**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A Novel Way to Immobilize Bacteriophage onto a Detection Platform with a Click

<u>KANGBENEDICTJM</u> 이효진[1] 최상기[2] Ralph Weissleder[3] 김은하[2,*]

아주대학교 분자과학 기술연구센터 [1]한국과학기술연구원(KIST) 생체재료연구단 [2]아주대학교 분자과학기술학과 [3]Harvard Medical School, USA

For last decade, bacteriophage has been used a useful material for applications other than for microbiology study.1 Owing to its high mutability, bacteriophages have been subjected to engineering for therapeutic and diagnostic purposes. Display technology was developed by using bacteriophage M13 to discover specific antigen peptide from a variety of candidates. Not only to an application for antigen discovery, recent engineering advancement has paid more attention to the bacteriophage's ability to selectively a target host. Bacteriophage as a binding element with an affinity offers a promising application in biosensor development for bacterial detection. There have been several studies that used bacteriophages for biosensors by physically immobilizing on solid platforms. It owes to surface chemistry to immobilize the virus to develop a biosensor, however, the whole process is often laborious and time consuming. Herein, we show a fast, chemoselective, covalent conjugation method for a new way to immobilize bacteriophage on a surface for biosensor development.

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장소: 일산 KINTEX
발표코드: **MAT.P-414**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Direct growth of graphene on SiO2 substrate using polyimide

신현석* 남한재[1]

UNIST 화학과 [1]UNIST 에너지공학과

AbstractSince graphene was first produced in laboratory, graphene has been regarded as a next-generation material due to its outstanding properties such as flexibility, high carrier mobility and transparency. Well-known graphene synthesis method is growth on metal-catalyst substrate such as copper and nickel with gaseous precursor. However, it should be required additional transfer process for applying electronic devices. The transfer process causes damage of graphene like polymer contaminants or defects to degrade its electronic property. Herein, we report growth of a few layer graphene on SiO2 substrate directly using 3,3’,4,4’-benzophenone tetracarboxylic dianhydride p-phenylenediamine (BTDA-PDA), not gaseous precursor i.e., CH4, and C2H4. BTDA-PDA is one of polyamic acid and can be converted to polyimide through imidization process. BTDA-PDA monolayer was coated on SiO2 substrate by Langmuir-blodgett whose method is helpful to control the number of polymer layer. We put copper foil on the sample, which has catalytic effect to form graphene. The Cu/BTDA-PDA/SiO2 was heated to 240 oC for imidization and 1070 oC for graphitization. Graphene was characterized by Raman spectroscopy and scanning electron microscope (SEM). The average intensity ratio I2D/IG is ~1.2. The coverage of BTDA-PDA derived graphene was confirmed ~70% by SEM and optical image.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-415**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Conversion of h-BN to graphene depending on different platinum orientation

김민수 신현석*

UNIST 화학과

Hexagonal boron nitride (h-BN)/graphene heterostructures exhibit several unusual properties that make them promising research for 2D materials. So far, in-plane h-BN/graphene heterostructures have been successfully realized through heteroepitaxial (or sequential) growth and patterned regrowth methods. Recently, we have developed a growth method to use conversion reaction on the metal substrate to directly convert h-BN to graphene. In the conversion process, we proposed Pt metal substrate plays a catalytic role and this reaction proceeds through h-BN hydrogenation; subsequent graphene growth quickly replaces the initially etched region.[1] However, a study on the interaction between h-BN and Pt metal has not been investigated in the conversion reaction. Here, we demonstrate the conversion rate of h-BN to graphene on the different Pt orientation. We observed (100) oriented Pt crystal shows the fastest conversion rate compared to (110) and (111) by SEM image. To investigate intermediate progress of conversion, we observed hydrogenation etching is huge difference according to Pt orientation by XPS measurement and inferred that hydrogenation is dominant factor for conversion of h-BN to graphene.Reference, [1] Kim, G.; Lim, H.; Ma, K. Y.; Jang, A.-R.; Ryu, G. H.; Jung, M.; Shin, H.-J.; Lee, Z.; Shin, H. S., Catalytic Conversion of Hexagonal Boron Nitride to Graphene for In-Plane Heterostructures. Nano letters 2015, 15 (7), 4769-4775.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-416**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synergistic effect of UV light shielding ability of bemotrizinol and mesoporous TiO_2 composite

박수빈 LICHENGBIN 이정호 김민지 김지만*

성균관대학교 화학과

Ultraviolet ray has very high energy to destroy chemical bonds, thus, it damages on DNA, human and animal tissues, other components under the skin, etc., easily. In order to protect our skin from UV light, researchers have developed various organic and inorganic sunscreening materials. Organic molecule exhibits very high UV light absorption ability, however, it has the potential to cause skin irritation, a respiratory ailment, and other diseases. Due to this, inorganic materials are used in the present. In case of inorganic material, it covers the surface of skin and reflects the lights irradiated. Therefore, it is less harmful than organic material. However, it is more difficult to put on inorganic sunscreen than organic one. Therefore, we investigated to use the advantages of both organic and inorganic materials. Currently, for UV-A and B blocking, organic and inorganic sunscreens were mixed physically and formulated. This process is easy to produce sunscreens, but it has disadvantages; difficulty of applying evenly, separation of materials, etc. In order to overcome those disadvantages and protect skin from UV-A and B both, the study of organic-inorganic composite materials for UV-A, B blocking was investigated.In this study,we have synthesized mesoporous TiO_2 with high surface area. For UV-A and UV-B blocking materials, we have studied to synthesize mesoporous TiO_2 impregnated with bemotrizinol which could block UVA light. The composite material exhibited higher UV shielding ability than physically mixed materials or each material alone. The synergistic effect of organic-inorganic composite was explored using computer-based simulation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-417**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The Phase transition and thermochromic characteristics of W/Nb-codoped VO_2(M) nanoparticles and its thin films

김종민 정영희[1] 심현관 김영일*

부경대학교 화학과 [1](주)마프로 기술연구소

VO_2(M) is a typical thermochromic material that has a property of changing near infrared (NIR) transmittance through the phase transition at about 68 ℃. This property has been widely studied for smart window application. However, its transition temperature(T_c) is pretty high to be applied for smart window, and several metal ions such as W, Nb, Mo were adopted for decreasing T_c as dopants. Among them W was well known as one of the most effective dopant for decreasing T_c with the rate of ca. 20 ℃ per W at.%. However, as the content of W increased, the transition sharpness was reduced and NIR switching efficiency in films therefore decreased.In this study we have investigated, for the first of time, the codoping of W and Nb into VO_2(M). First, we synthesized W/Nb-codoped VO_2(M) nanoparticles by the hydrothermal and post thermal treatment method and prepared its thin films by a wet-coating method from its solvent-dispersed coating solution. W/Nb-codoped VO_2(M) showed a relatively good transition characteristics as well as reduced T_c compared with only W-doped one. And its thin films showed much better NIR switching efficiency with reduced T_c.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-418**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Comparison of 1T and 2H phase MoS_2 by surface functionalization with methoxy benzene diazonium salt

장윤정 신현석*

UNIST 화학과

Functionalization of MoS_2 is studied in these days because electric property of MoS_2 can be modified by various functional group. However, mechanism of functionalization of 1T-MoS_2 and 2H-MoS_2 is still unknown so comparing functionalization form of 1T and 2H phase MoS_2 can give clue of functionalization mechanism. 1T-MoS_2 has negative surface charge and 2H-MoS_2 has neutral surface charge. Because 1T phase and 2H phase have different surface charge, bonding with MoS_2 and functional group would be different. From this reason, functionalization of 1T-MoS_2 and 2H-MoS_2 is expected to be different using same functional group, methoxy benzene diazonium tetrafluoroborate (MB diazonium salt). Based on our expectation, we investigated bonding mechanism of functionalized 1T and 2H MoS_2 in our research. MB diazonium salt is reacted with dispersed 1T-MoS_2 in water and dispersed with 2H-MoS_2 in NMP for 1 day, respectively. 1T-MoS_2, 2H-MoS_2, methoxybenzene-1T-MoS_2(MB-1T-MoS_2), and methoxy benzene-2H-MoS_2 (MB-2H-MoS_2) are characterized by Scanning electron microscope, zeta potential, and, Fourier transform infrared spectroscopy. S-C covalent bonding between 1T-MoS_2 and MB diazonium salt is characterized by X-ray photoelectron spectroscopy (XPS), while physisorption of MB diazonium salt on 2H-MoS_2 is confirmed by XPS.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-419**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Paper-based Digital Microfluidic Chip Goes for Gold Nanorod Synthesis Thereof

정해나 김윤표 권오선[*] 신관우[1,*]

서강대학교 화학과 [1]서강대학교 화학과 및 바이오융합과정

To complete the gold nanoparticle synthesis in electromicrofluidics by varying critical parameters such as volume, thermal, and chemical ingredient quantities, three major elements of dispenser, heater and temperature sensor have been integrated on a paper-based active digital microfluidic (DMF) chip platform. The dispenser was composed of a reservoir, an opening gate and an array of electrodes providing that a series of digital drops were generated out of each of reservoirs by electrowetting force. So simple, easy and quick drop generation enabled the easy drop manipulation in a digital unit to replace the flow based in tedious numerous and spatial pipetting and vial lab-work. The micro heater allowed the endothermic reaction, and a temperature sensor monitored the drop and the heater temperature. Printing method was used for fabrication of the patterned electrode of DMF chip plate which was required for electowetting driven drop actuation actively as well as three elements, with conductive silver nanoparticle ink charged on an office inkjet printer. Additionally, the electronic plotter was used for mechanical cutting of Scotch tape for a dispenser well. Before investigation of variations of gold nano-rod formation by varying parameter, such as thermal effect, dispersant and precipitation concentrations, various characteristic electromicrofluidic, chemical and thermal performance and responses of three elements have been studied by using infrared imaging camera, SEM, AFM, vis-UV and FTIR spectroscopies. Selected experimental results are: 1) the droplets dispense showed linear behavior between the applied voltage and the dispensed droplet size. 2) Gold nanorods appeared with aspect ratios of 1.3, 10.1, 17.8.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-420**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Polydopamine Coated Layered Double Hydroxide and its Silver Metal Nanocomposites

이용주 정덕영*

성균관대학교 화학과

A novel hybrid of silver deposited polydopamine/layered double hydroxide nanocomposite(PDA/LDH) was synthesized. Polydopamine(PDA) was deposited on layered double hydroxide(LDH) through an interlayer polymerization(PDA/LDH). Kinetic controlled polymerization of dopamine in basic buffer solution under a nitrogen atmosphere provided a synthetic pathway for the nanostructured PDA/LDH composites without polymer agglomerates. We synthesized the silver coated-PDA/LDH and found the novel nanostructures of deposited silver metals. The simple method demonstrated to control the silver nanoparticle density and morphology onto the polydopamine coated LDH. In order to control silver deposition and its morphology, the experimental parameters including silver reduction time, UV light radiation, thermal treatment were investigated. The optimized samples demonstrated remarkable surface-enhancement ability in Raman scattering signals. PDA coating not only serves as a reducing agent for the deposition of silver nanoparticle on LDH in a controlled manner, but also contributes to the observed Raman scattering in terms of improving photon scattering and promoting electron transfer processes.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-421**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Crystal Structure of Zinc Hydroxide

박용민 정덕영*

성균관대학교 화학과

The layered compound, zinc hydroxide nitrate ($Zn_5(OH)_8(NO_3)_2 \cdot 2H_2O$) that was harmless to humans, was usually researching for catalyst’s support or drug delivery system’s carrier. We synthesized the layered zinc hydroxide nitrate in aqueous solution, which was characterized by Raman spectrum, X-ray diffraction and Fourier transform infrared spectroscopy

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장소: 일산 KINTEX
발표코드: **MAT.P-422**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

One-Pot Synthesis and Thin Film Deposition of $Co(OH)_2$ Single-Layer Nanosheets

정선호 정덕영*

성균관대학교 화학과

$Co(OH)_2$ single-layer nanosheets were prepared by a facile one-pot synthesis, and directly deposited on nickel foam by electrophoretic deposition. Formamide was used as a solvation reagent to prevent $Co(OH)_2$ single-layers from stacking while $CoCl_2$ precursor was dissolved in distilled water. The pH value of $CoCl_2$ precursor solution was increased by ammonia gas transfer method in an enclosed system. The size of as-prepared $Co(OH)_2$ single-layers was 200 nm with low deviation and amorphous crystallinity which were analyzed by TEM, UV-vis, DLS, SEM, and XRD measurements. Nickel foam was dipped into the $Co(OH)_2$ single-layer solution and $Co(OH)_2$ thin film was rapidly fabricated in parallel with the nickel metal surface by low applied voltage, showing 3150 Fg^{-1} specific capacitance at 2 Ag^{-1}.

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장소: 일산 KINTEX
발표코드: **MAT.P-423**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Improved Survival and Patterned Growth of Neurites on Microscale Laser-scribed rGO film

이한별 강경태*

경희대학교 응용화학과

Graphene has gained spotlight as a next generation material, due to its flexibility and great conductivity. By using a recently developed laser scribing method using a DVD disc, we fabricated reduced graphene oxide (rGO) film, and tested its compatibility for primary hippocampal neuron culture. The rGO film interestingly had good biocompatibility without any neuro-adhesive coating (e.g., poly-D-lysine), while neurons were barely found on GO substrates, making a large contrast between the two surfaces. In addition, intrinsic circular line patterns of rGO made during the laser-scribing effectively guided neurite outgrowth, making the neurons stretch their neurites linearly along the lines of laser-scribed rGO. We attribute this neurite guidance effect to the rough surface topography of rGO generated during the laser treatment. In summary, we suggest that our new method can be a facile and versatile method for the large-scale generation of neuro-compatible and neurite-guiding substrates, which will have numerous biomedical applications including biochips for studying human diseases.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-424**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

In vivo compatibility of chitosan-hydroxyapatite composite film depending on degree of deacetylation

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

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-425**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Heteroatom Doped Ordered Mesoporous Carbon for Supercapacitors

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성균관대학교 화학과

Supercapacitors (SCs) have been widely studied around the world in recent years, due to their excellent power density and long cycle life. As the most frequently used electrode materials for SCs, carbonaceous materials attract more and more attention. However, their relatively low energy density still holds back the widespread application. Up to now, various strategies have been developed to improve the SCs performance of carbonaceous materials, including the incorporation of heteroatoms and the pore size effect. In this work, nitrogen and phosphorous co-doped ordered mesoporous carbons (OMCs) have been synthesized by nanocasting method using KIT-6 (Ia3d) as a hard template. In addition, the texture and surface properties are strongly dependent on the carbonization temperature. Cyclic voltammetry tests have been used to investigate the capacitive performance of such carbon materials, which exhibit high specific capacitance.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-426**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

In vivo feasibility test of nerve regeneration with carbon nanotube-coated polydimethylsiloxane sheet

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Carbon nanotubes (CNTs), with their unique and outstanding properties, such as strong mechanical strength and high electrical conductivity, have become very popular for the repair of tissues, particularly for those requiring electrical stimuli. Polydimethylsiloxane (PDMS)-based elastomers have been used in a wide range of biomedical applications because of their optical transparency, physiological inertness, blood compatibility, non-toxicity, and gas permeability. In present study, most of artificial nerve guidance conduits (ANGCs) are not transparent. It is hard to confirm the position of two stumps of damaged nerve during nerve surgery and the conduits must be cut open again to observe regenerative nerves after surgery. Thus, a novel preparation method was utilized to produce a transparent sheet using PDMS and multi-walled carbon nanotubes (MWNTs) via printing transfer method. Characterization of the PDMS/MWNT (PM) sheets revealed their unique physicochemical properties, such as superior mechanical strength, a certain degree of electrical conductivity, and high transparency. Characterization of the in vitro and in vivo usability was evaluated. PM sheets showed high biocompatibility and adhesive ability. In vivo feasibility tests of rat brain tissue and sciatic nerve revealed the high transparency of PM sheets, suggesting that it can be used in the further development of ANGCs.

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발표코드: **MAT.P-427**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Comparison of Physical and Chemical Behavior of Sulfur Mustard (HD) Removed Using Different Sorbents

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Chemical warfare agents (CWAs) are chemical substances whose toxic properties are used to kill, injure or incapacitate human beings. Thus, decontamination, aimed at eliminating the hazard of CWAs, is important and required on the battlefield as well as in laboratories, pilot plants, and chemical agent production, storage, and destruction sites. Among them, the majority of research is focused on battlefield conditions where speed and ease of application of the decontaminant are essential. Battlefield decontamination is the rapid removal of chemical agents from military vehicles, equipment, personnel, and facilities by both chemical and physical methods. Consequently, a solid surface on which chemical agents are deposited is the primary target for decontamination. In this study, a test on the removal of sulfur mustard (HD) from CARC (Chemical Agent Resistant Coating) specimens with two different solid sorbents was performed, and the decontamination efficiency was investigated by using mass-spectroscopic and gas-chromatographic techniques. The details of the physical and chemical behavior of HD according to the type of sorbent in the decontamination process will be presented.

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발표분야: 재료화학
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Tailoring of Eu-doped YVO_4 nanoparticles on the LYH films for detection and removal of Cu^{2+} cations in water

김현섭 변송호*

경희대학교 응용화학과

Human body requires metallic elements such as copper that are vital for normal metabolic processes. Nonetheless, monitoring of Cu^{2+} is essential since too much intake can affect one’s health to cause diarrhea, vomiting, stomach cramps, and nausea, and may lead to life threatening illnesses such as liver damage and kidney disease. The world’s health governing bodies limit the drinking water Cu content to 31.5 μM. Accordingly, it is imperative to detect its presence as well as to eliminate Cu so as to maintain its concentration lower than the standard level. We previously reported that Eu-doped YVO_4 (YVO_4:Eu) nanoparticles, prepared in aqueous solutions at room temperature, have high affinity towards Cu^{2+} ions. Such a behavior can be the basis on developing an alternative method for copper detection and elimination. In this work, chemical bath deposition (CBD) technique was used to deposit Eu-doped LYH films on glass substrates. The reaction of resulting films in aqueous $NaVO_3$ solutions produced a new type of film, where YVO_4:Eu nanoparticles are tailored at the edge of LYH nanosheets. As predicted, a strong red color emission was observed when the as-prepared Eu-doped YVO_4/LYH film was irradiated by UV. In contrast, the emission intensity diminished considerably after the adsorption reaction in aqueous Cu^{2+} solutions. The intensive adsorption of Cu^{2+} cations on the film surface occurred via the electrostatic interaction owing to the negative surface potential of YVO_4:Eu nanoparticles. Thus, the complementary overlap of the emission band of YVO_4:Eu with the absorption band of Cu^{2+} results in an effective filter effect to induce the distinct fluorescence quenching. Considering easy deposition of Eu-doped YVO_4/LYH films on various shapes of glass substrate such as plates, walls, containers, or tubes, our approach demonstrates a promising technique for the monitoring and elimination of Cu^{2+} ions in environmental waters.

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발표코드: **MAT.P-429**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Phosphate uptake behavior of luminescent layered yttrium hydroxide in aqueous solutions

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Phosphorus is an essential nutrient element for all living organisms and its application in agriculture as a fertilizer is important for production of food. In contrast, an excess phosphate can cause serious eutrophication of lakes, reservoirs, estuaries, and parts of the oceans. Considering that only 1/5 of applied phosphate fertilizer is incorporated into the foods of plants and animals that humans consume, most of phosphorus is lost along the way of flow through the food production and consumption system. Therefore, a special interest is required to develop efficient materials able to recover or remove the phosphate from environment water body. In this work, the layered yttrium hydroxide (LYH), $Y_2(OH)_5Cl \cdot nH_2O$ was prepared at room temperature in aqueous solutions and its adsorption behavior of phosphate was investigated. LYH was found to have high anion uptake capacity that enhances its capability to remove anionic contaminants from aqueous system. In particular, we have found that P at a concentration below 5 ppm can be very efficiently and quickly removed through complexation on the LYH particle surface, with less than 0.3 ppm of P left in solution. When Ce^{3+} was doped, the blue-emission from Ce-doped LYH could be employed to detect the phosphate in aqueous solutions. Therefore, LYH is a potential cost-effective adsorbent for trace phosphate. Furthermore, the analyses of the uptakes in mixed aqueous solution containing NO_3^-, CO_3^{2-}, and SO_4^{2-} showed that the adsorbent had a markedly high selectivity for the adsorption of phosphate ions.

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발표코드: **MAT.P-430**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Modification of a facile hydrothermal method for upconversion enhancement of $NaYF_4$: Yb^{3+}/ Er^{3+}, UCNPs and exploring the hidden dimensions

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중앙대학교 화학과

Upconversion nanoparticles (UCNPs) have several unique properties that make them appropriate for use in multiple fields. In this work, we optimized a facile hydrothermal method to tune the size, crystal phase, homogeneity as well as UC luminescence of $NaYF_4$: Yb^{3+}, Er^{3+}. Characterization of the synthesized nanocrystals was done by scanning electron microscope (SEM), high-resolution transmission electron microscope (HRTEM), X-ray diffraction (XRD), photoluminescence (PL) and UV-visible absorbance spectra. The molar concentration and volume of NaF and reactants content were optimized first to obtain nanocrystals with good homogeneity, phase and luminescence. The reactants content represents the total quantity of Y^{3+} and doped lanthanide ions such as Yb^{3+} and Er^{3+}. After that, the concentration of Yb^{3+} and Er^{3+} ions were adjusted while keeping the molar concentration of NaF and reactants constant. To further investigate the best luminescence conditions, the hydrothermal reaction time was also optimized. It was found that optimization factors affect the shape of the resulting nanocrystals and phase transition from cubic to cubic and hexagonal and finally pure hexagonal phase. The results show that UCNP doped with 20% Yb^{3+}, 3% Er^{3+} and treated at 190°C for 7 h hydrothermal reaction time have good homogeneity, hexagonal phase and the highest luminescence intensity when excited by 980 nm laser diode. The as-prepared UCNPs can be well-dispersed in water without further surface modification. These water-soluble nanocrystals can be applicable in biological and medicine fields as imaging agents.

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발표코드: **MAT.P-431**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Adsorption reaction of phosphate anions with layered yttrium hydroxide

이현숙 김현섭 변송호*

경희대학교 응용화학과

In an attempt to develop a new adsorbent with high phosphate uptake capacity, the layered yttrium hydroxide (LYH), $Y_2(OH)_5Cl \cdot nH_2O$, has been prepared using hexamethylenetetramine ($(CH_2)_6N_4$; HMTA) under ambient pressure. The adsorption reaction of phosphate anions was successfully carried out in the gallery and surface of LYH. Because phosphate ions exist in different ionic states, H_3PO_4, $H_2PO_4^-$, HPO_4^{2-}, and PO_4^{3-}, the ion-exchange reactions were performed at different solution pHs (6, 7, and 8) and consequently measured phosphorus uptake capacity of LYH were significantly different depending on the initial pH of aqueous solution. These values are compared with calculated maximum phosphorus uptake capacities, supposing a complete 1:1, 1:2, and 1:3 exchange between phosphate and Cl^- ions of LYH ($Y_2(OH)_5Cl \cdot 1.5H_2O$), respectively. For instance, the maximum uptake capacity of LYH is expected to be close to ~100 mg-P/g at pHs < 6. Based on the experimental observation indicating the occurrence of complete 1:1 exchange reaction between chloride ions and phosphate ions, a possible mechanism of phosphate uptake by LYH is proposed. No difference in XRD pattern of LYH before and after adsorption reaction at low pHs suggests also a possible adsorption through the ligand complexation on the particle surface.

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발표코드: **MAT.P-432**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Hydroxylated YVO_4:Eu; luminescent adsorbent for the detection and removal of Cu(II) in aqueous solutions

이성란 김현섭 변송호*

경희대학교 응용화학과

Copper that widely exists in nature can be readily absorbed and distributed all over the human body. For example, copper is stored in the brain, liver, kidney, heart, spleen, and blood in the human body, with the concentration ranging from ~1 to ~4 μg/g or μg/ml. An excess of copper can cause neurotoxicity through the deposition of Cu(II) in the lenticular nucleus of the brain and liver, which is often associated with kidney failure as well. In the present work, YVO_4:Eu nanoparticles induced from yttrium hydroxocation nanosheets and VO_3^- anions were used to remove Cu(II) from aqueous solution. The size of quite regular rice-like particles is controllable in 50 ~ 200 nm range by adjusting solution pH. Due to a large remnant of hydroxyl groups on their surface, YVO_4:Eu nanoparticles could be readily dispersed to form stable aqueous colloidal solutions without any additional surface modification. Adsorption kinetics of YVO_4:Eu nanoparticle in colloidal solutions containing Cu(II) have been examined and its adsorption isotherm was fitted with several models. The maximum copper adsorption capacity reaches up to 36 ~ 61 mg/g at 5 < pH < 9 and sensitive adsorption speed is demonstrated by the efficient filter effect of adsorbed Cu(II) to quench the emitted fluorescence light from YVO_4:Eu.

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장소: 일산 KINTEX
발표코드: **MAT.P-433**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis and UV-shielding property of ceria nanoparticles with Ce^{4+} – Ce^{3+} core-shell structure

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Cerium oxides, $CeO_{2-\delta}$, with mixed Ce^{3+}/Ce^{4+} oxidation states have attracted considerable attention in recent years due to their exceptional technological applications in oxygen storage capacity, catalyst, solid oxide fuel cells, dye removal treatments, and optical properties. In particular, due to its UV absorption in the harmful 210 – 310 nm region and low photocatalytic activity, $CeO_{2-\delta}$ is considered as a promising nanomaterial for use in sunscreens. In this work, large-scale production of regular $CeO_{2-\delta}$ nanoparticles (10 < d < 20 nm) was accomplished in aqueous solutions of $CeCl_3$ at room temperature. ($CeCl_3 \cdot 7H_2 0$ 5mmol were dissolved in 30ml deionized water. The KOH solution was then added drop-wise to the prepared solution.) Prepared nanoparticles with a lot of remnant surface hydroxyl groups were well dispersed to form aqueous colloidal solutions. The Ce^{3+}/Ce^{4+} ratio (i.e. δ value) was controlled with several reducing agents and ultimately to form Ce^{4+} – Ce^{3+} core-shell structured nanoparticles. Relationship between Ce^{3+}/Ce^{4+} ratio and UV-shielding ability was assessed using UV-vis reflectance and absorption technique. Practically, UV absorption of $CeO_{2-\delta}$ was not significantly influenced by the change of Ce^{3+}/Ce^{4+} ratio, indicating a potential application of Ce^{4+} – Ce^{3+} core-shell structure in sunscreens as well as antioxidants.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-434**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

N-doped Carbon and Reduced Graphene Oxide Dual Layer Coating on $LiFePO_4$ Nanoplates as High-Performance Lithium Ion Battery Cathode Material

오지섭 박원철*

서울대학교 융합과학기술대학원 융합과학부

Lithium ion batteries (LIBs) possess the 1st candidate for electrochemical energy storage devices. However, the improvement of energy density and power density of LIBs is still urgently required to match the market demands for electric vehicles (EVs) and hybrid electric vehicles (HEVs). Until now, many kinds of electrode materials for EVs and HEVs applications have been investigated. Among them, $LiFePO_4$ (LFP) has advantages, such as good thermal stability, abundant precursors, and high theoretical capacity. However, low lithium ion diffusivity and poor electric conductivity are major drawbacks of LFP, which limit its extending application. In this study, we report a dual carbon layer coating on LFP nanoplates as cathode material for LIBs.After careful comparison, we used polydopamine-derived nitrogen-doped carbon (N-doped carbon) and reduced graphene oxide (RGO) to coat LFP nanoplates. The dual carbon layer coated LFP exhibits a high rate performance (98 mAh/g at 30 C) and excellent long-term cycling stability (discharge capacity of 115 mAh/g at 10C, and 96.18% capacity retention after 700 cycles). This excellent performance can be attributed to (1) the conductive electron pathway along N-doped carbon on LFP nanoplates, (2) the connected conductive electrode with a well-knitted RGO network, and (3) the fast Li^+ ion diffusion induced by the small size of the nanoplates. The dual layer coating with polydopamine derived N-doped carbon and RGO is expected to be a good strategy for enhancing the performance of electrode materials for LIBs.

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장소: 일산 KINTEX
발표코드: **MAT.P-435**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Size-controllable and scalable synthesis highly uniform silica nanoparticles in alkaline buffer solution and its application for efficient sentinel lymph node imaging

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Nanomaterial-based anti-cancer medicine is an active field of nanoscience for enhancing the therapeutic and diagnostic efficacy in clinical area. Here, a scalable synthesis of highly monodisperse small silica nanoparticles with wide size-range was achieved via fine tuning of reaction temperature in various alkaline buffer solutions as catalysts. Having shown the ability to precisely synthesize size controlled silica nanoparticles with fluorescence labelling process, we performed in vivo fluorescence imaging and immunofluorescence analysis of sentinel lymph nodes (SLNs) with the nanoparticles having different sizes to investigate the size-dependent effect for SLNs identification. The 12 nm-sized nanoparticles showed effective SLN uptake within 10 min after intradermal injection and were evenly localized inside the SLN, whereas the 120 nm-sized nanoparticles failed to identify the SLN and distributed only in the medulla region not in the superficial cortex of the SLN. Taken together, a new facile scalable synthesis technique for fine size controlling of silica nanoparticles was developed and it made possible to find the optimized size of nanoparticles for efficient SLN mapping.

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발표분야: 재료화학
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Dielectric and electrical properties of $Y_{2/3}Cu_{2.90}Zn_{0.10}Ti_4O_{12}$ polycrystalline material

SINGHLAXMAN 이영일*

울산대학교 화학과

Zn doped $Y_{2/3}Cu_{2.90}Zn_{0.10}Ti_4O_{12}$(YCZTO) material has been synthesized. The X-ray diffraction analysis showed the single phase formation of the YCZTO material sintered at 1050 °C for 15 hrs. Scanning electron microscopy (SEM) showed well packed grains having the average grain size in range of ~0.8–4 μm. Energy dispersive X-ray spectroscopy (EDX) results reveal the presence of the elements yttrium, copper, zincs, titanium, and oxygen and thus justifying the purity of the synthesized material. YCZTO exhibited the high dielectric constant (ε_r) value of ～1.4 x10^3 and low dielectric loss (tan δ ～.09) at 50 °C. The impedance spectroscopy analysis suggested that the obtained YCZTO material is electrically heterogeneous. The activation energies (E_a) for grain boundaries at higher temperature range (383-403 °C) were found to be in the range 1.0 eV.

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장소: 일산 KINTEX
발표코드: **MAT.P-437**
발표분야: 재료화학
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A facile ultrasonic-assisted fabrication of carbon nitride/carbon dots composites for photocatalytic degradation behaviors of rhodamine B

장익범 박수진[1,*]

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The novel visible light-induced carbon nitride/carbon dots ($g-C_3N_4$/CDs) composites were successfully synthesized by introducing CDs into polymeric $g-C_3N_4$. 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 $g-C_3N_4$/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 $g-C_3N_4$/CDs was proposed to guide the further improvement of their photocatalytic activity.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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A Facile Route to Aziridine-Functionalized Polydimethylsiloxanes for Tailorable Polymeric Scaffolds

강서현 박소현 최윤수 윤효재*

고려대학교 화학과

This presentation will describe a facile and efficient method to construct tailorable polymeric scaffolds on a molecular scale through the ring opening reaction of three-membered N-heterocyclic compound, aziridine. Aziridine is incorporated into elastomeric polymer backbone (polydimethylsiloxane; PDMS) through Pt(0)-based hydrosilylation reaction. The resulting polymers (denoted as aziPDMSs) retain attractive features such as optical transparency and elastic property as compared to conventional PDMS. Post-modification of aziPDMS is achieved through orthogonal ring opening reaction of the aziridine pendants. The manufacturing process and structural modification reaction are straightforward and effective, and can be carried out with commercially available reagents (prepolymers) without further processes.

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In-situ synthesis of BiOClx/BiOBry/BiOIz nanofibers for visible-light photocatalytic investigation

장익범 박수진[1,*]

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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: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-440**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

In-situ growth of Graphene Oxide/BiOCl composites nanofibers and their application in photocatalytic degradation of RhB

장익범 박수진[1,*]

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In this paper, we prepared the graphene oxide/BiOCl/PAN nanofibers by two-step synthesis method and characterized their structures, morphologies, and photocatalytic behaviors by X-ray diffraction, diffuse reflectance spectroscopy, scanning electron microscopy and photocatalytic activity measurements, respectively. From the results, we can obtain that coupling graphene oxide/BiOCl fibers could enable better photocatalytic performances as compared to that pure BiOCl towards the degradation of rhodamine B under visible light irradiation. It could be attributed to the more effective separation of photogeneration electron and holes between BiOCl and graphene oxide, and the better adsorption capacity of rhodamine B.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-441**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

New cathode material for magnesium ion battery : NbSe2

유제인 형주은 홍승태*

DGIST 에너지시스템공학

Rechargeable magnesium-ion batteries have received attention as one of the candidates for next-generation electrochemical energy storage. The magnesium-ion batteries have advantages such as lower cost and higher energy density, compared with lithium-ion batteries. Moreover, they are safer due to the absence of dendrite problems. Despite such advantages, few cathodes have been reported for the magnesium-ion batteries.Herein, we report a new cathode material, NbSe2 (hexagonal, P63/mmc, a = 3.4439 Å c = 12.53980 Å V = 128.8019 Å3), for the magnesium-ion aqueous battery. Metal selenide-based materials have lower electronegativity than oxygen. So, it is better for magnesium-ion diffusion. And aqueous system, is cheaper than organic system that using organic solvent. Therefore, we suggest NbSe2 for aqueous magnesium-ion battery cathode material.Detailed analyses with ICP-OEC, EDX, XRD were performed to confirm the Mg ion intercalation chemistry. This result should be an important basis for understanding the electrochemical intercalation reaction of magnesium as well as other divalent ion into various host materials.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-442**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of Stretchable and Flexible Graphene-based Supercapacitors using PDMS

정예빈 이민형*

경희대학교 응용화학과

There are many recent studies of wearable technologies and devices that stretchable and flexible. Stretchable and flexible supercapacitors are essential component of pliable electronic devices. Therefore, we fabricated flexible and stretchable supercapacitor by simple process. Polydimethylsiloxane(PDMS) was appropriately synthesized on a silicon wafer through a spin coating process and cured in an oven at 150℃ for 7 hours. Then a solution containing graphite oxide(GO) was dispersed on the surface of the wafer. In this work, we used Polydimethylsiloxane(PDMS) as a substrate that has a hallmark of elasticity. Moreover, the surface area was manipulated by using LightScribe DVD that laser directly reduces the graphite oxide(GO) films to form graphene oxide(rGO).

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-443**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrochemical Behavior of RGO/N-doped Carbon form/Sulfur Nanocomposite as a Cathode in Lithium-sulfur Batteries

이정연 박원철*

서울대학교 융합과학기술대학원 융합과학부

Heteroatom doping of carbon materials has been an important method to further improve the electrochemical performance in lithium-sulfur batteries owing to capping effect by strong interaction between heteroatom and polysulfides. However, general processing of heteroatom doping is still challenging due to high toxicity and complexity during the doping process.In this study, by using commercial melamine foam with about 8wt% of nitrogen, high N-doped carbon framework loaded with graphene was prepared by a simple heat treatment method and used as a reservoir of sulfur cathode in lithium-sulfur batteries. The electrode of RGO/N-doped carbon framework/Sulfur indicates an initial capacity of about 1361 mA h g^{-1} at 0.1 C, and maintains a specific capacity of about 631 mA h g^{-1} after 150 cycles at 0.5 C. The improved cycling stability and high efficiency are attributed to the capping effect exerted by N-doping for polysulfides and high electrical conductivity of the carbon framework.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-444**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

A new host material in Ba-V-O system with an unprecedented crystal structure for rechargeable multivalent-ion batteries, synthesized by an electrochemically-supported reaction

곽헌호 홍승태*

DGIST 에너지시스템공학

Discovery of new inorganic ceramic materials has been always challenging, and has led a major breakthrough in material science. In this work, an unprecedented material was discovered in Ba-V-O (BaVO). It was synthesized by an electrochemically-supported synthetic method. The material showed excellent electrochemical intercalation of multivalent ions, such as Mg, Ca and Ba ions. We discovered a quick synthetic method to prepare the BaVO from $Na_{1.2}V_3O_8$, utilizing a simple electrochemical reaction. The electrochemical multivalent ion intercalation into the BaVO was confirmed by cyclic voltammetry, galvanostatic discharge/charge, powder XRD and elemental analyses. Reversible redox reactions were observed in cyclic voltammograms as well as discharge/charge cycles, which is responsible for the intercalation of the guest ions.We demonstrated the a successful multivalent ion intercalation into the BaVO host material, and new crystal structures of BaVO and multivalent-inserted BaVO have been determined for the first time by this work through the techniques of structure determination from powder X-ray diffraction data.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-445**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Nickel Hexacyanoferrate as a Cathode Material for Magnesium-ion Batteries

채문석 형주은 홍승태[*]

DGIST 에너지시스템공학

The organic electrolyte-based rechargeable magnesium-ion battery (MIB) demonstrated utilizing Prussian-blue (PB) analogue potassium nickel hexacyanoferrate K0.86Ni[Fe(CN)6]0.954(H2O)0.766 (KNF-086) as the cathode material. The KNF-086 cathode is prepared via electrochemical extraction of potassium ions from K1.51Ni[Fe(CN)6]0.954(H2O)0.766 (KNF-151). The electrochemical cell is composed of a KNF-086 cathode, an activated carbon anode, and a 0.5 M Mg(ClO4)2 acetonitrile electrolyte. This cell shows a reversible discharge capacity of 48.3 mAh g−1 at 0.2 C rate with the discharge voltage at 2.61 V (vs. Mg2+/Mg). As evidenced by Fourier electron density analysis with powder XRD data, the magnesium-inserted phase is confirmed as Mg0.27K0.86Ni[Fe(CN)6]0.954(H2O)0.766 (MKNF-086), and the position of the magnesium ion in MKNF-086 is revealed as the center of large interstitial cavities of the cubic PB. Compared to KNF-086, MKNF-086 exhibits a decreased unit cell parameter (0.8%) and volume (2.4%). The elemental analysis indicated that magnesium-ion was inserted/extracted as the guest-ion during discharge/charge process. Our result shows great promise for the organic electrolyte-based MIB with the non-aqueous and non-Grignard electrolytes, and offers a crucial basis for understanding the electrochemical intercalation chemistry of magnesium ions in the general organic electrolyte.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-446**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

$MgV_6O_{16}\cdot 9H_2O$: a new positive material for lithium-ion batteries, synthesized by a electrochemically-supported reaction

김효정 곽헌호 홍승태*

DGIST 에너지시스템공학

We report a novel electrochemical synthesis of a hydrated mineral $MgV_6O_{16}\cdot 9H_2O$ by using LiV_3O_8 as a precursor which was prepared via the solid-state reaction method. Herein, we demonstrated firstly the possibility of the electrochemically synthesized $MgV_6O_{16}\cdot 9H_2O$ material for the positive electrode of lithium ion batteries (LIBs), which clearly showed the intercalation of Li^+ to the host $MgV_6O_{16}\cdot 9H_2O$. The electrochemical Li^+-intercalation was confirmed by cyclic voltammetry (CV), galvanostatic discharge/charge cycling, powder X-ray diffraction (XRD), and energy dispersive X-ray spectroscopy (EDX). Reversible reduction and oxidation peaks were observed on CV curves as well as discharge/charge cycling data. The crystal structures of $MgV_6O_{16}\cdot 9H_2O$ and the Li-inserted form, $Li_xMgV_6O_{16}\cdot 9H_2O$, were unknown and characterized for the first time through the structure determination from powder XRD data to understand the Li^+-intercalation mechanism in more detail.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-447**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Investigation of birnessite as a calcium-ion energy storage system

형주은 허종욱 곽헌호 채문석 홍승태*

DGIST 에너지시스템공학

The concept of Ca-ion battery (CIB) is just in its infancy, as one of the post Li-ion batteries. The prepared layered birnessite (δ-MnO_2) was characterized as a cathode material for CIBs. Cyclic voltammetry (CV) and galvanostatic experiments showed reversible calcium insertion/extraction reactions into/from the birnessite, which was also evidenced by XRD and elemental analyses. Kinetic analysis based on CV with various scan rates indicated that both the intercalation and pseudo-capacitance are responsible for the reaction. This work demonstrates that the birnessite can be a cathode material, and also offers the possibility of discovering other new electrode materials for CIBs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-448**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High-Voltage K-ion Batteries using Zn/Fe-based Rhombohedral Prussian blue analogue

허종욱 채문석 형주은 홍승태*

DGIST 에너지시스템공학

Potassium-ion batteries (PIBs) have received attention as a new-type energy storage system, which has potential advantages as an abundant element and expected lower cost. Despite the several advantages, a little is known about cathode materials for KIBs especially in organic electrolyte systems. Herein, we studied and constructed a high voltage rechargeable PIBs using metal organic framework, rhombohedral Prussian blue (RPB) analogue potassium zinc hexacyanoferrate $K_{1.88}Zn_{2.88}[Fe(CN)_6]_2\cdot 5H_2O$ (KZnHCF) as a cathode material. Two different kinds of KZnHCF were prepared via simple precipitation method– nanocube (C-KZnHCF) and irregular (I-KZnHCF) particle shape. The cell is composed of a KZnHCF cathode, a potassium metal anode, and a 0.5 M KPF_6 in EC/DEC electrolyte. We focused on its electrochemical properties and structural changes during the potassium intercalation. The first discharge capacity was 55.6 mAh/g with an average operating voltage of 3.9 V vs. K/K^+. The capacity retention at the 100th cycle was 95% (C-KZnHCF) and 88% (I-KZnHCF) versus the first discharge capacity, respectively. The reversible insertion/de-insertion reaction of potassium into the structure of KZnHCF was clearly evidenced by the elemental analyses and electron density mapping of the structure using the techniques of structure determination from powder X-ray diffraction data. This result can strongly contribute to the development of organic electrolyte based PIBs as energy storage systems, and offers a crucial basis for understanding the electrochemical intercalation chemistry of potassium ions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-449**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrochemical magnesium ion intercalation into $Na_3V_2(PO4)_3$ as a cathode candidate for Mg batteries

전부식 허종욱 홍승태*

DGIST 에너지시스템공학

Magnesium-ion secondary batteries (MIBs) have attracted attention as an alternative to lithium-ion batteries. This is because MIBs have some advantages over lithium-ion batteries such as lower cost, higher energy density, and more abundance than lithium. In addition, MIBs are expected to have higher safety due to the characteristic of magnesium on which dendrite does not grow well. With these advantages, researches on cathode materials and electrolytes suitable for MIBs are actively underway. Herein, we report a remarkable cathode material for MIBs, Nasicon-type structure $Na_3V_2(PO_4)_3$ (Rhombohedral, R-3cH, a = 8.73 Å c = 21.81 Å V = 1438.73 Å^3), in an aqueous system. The rhombohedral $Na_3V_2(PO_4)_3$ has three dimensional framework and large interstitial sites allowing easy transportation of magnesium ions through the channels. In addition, the aqueous system could be cheap and environmentally friendly. In this work, we demonstrate that $Na_3V_2(PO_4)_3$ can be a feasible host material for aqueous MIB.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **MAT.P-450**

발표분야: 재료화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

M13 박테리오파지를 이용한 구조색 컬러 디스플레이

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구조색을 이용한 반사형 디스플레이는 기존에 개발된 디스플레이가 가지지 못하는 다양한 장점들로 최근 많은 주목을 받고 있다. 대표적으로 후광 없이 작동 가능해 낮은 전력 소모를 보인다는 점, 일반적인 디스플레이에 비해 간결한 제조 과정을 통해 제조 가능하다는 점 등을 들 수 있다. 이에 따라 많은 연구자들이 콜레스테릭 액정 디스플레이, 쌍안정 네마틱 액정 디스플레이, 전기 영동 디스플레이, 간섭 측정 변조기 디스플레이 등의 다양한 반사 디스플레이들을 연구해 왔다. 본 연구진은 M13 박테리오파지가 액정과 비슷한 특징을 가진다는 점을 보고하였다. 박테리오파지가 가지는 자기 진화, 자기 복제, 자기 배열 등의 특징은 많은 응용분야에 적용이 가능할 것으로 예상된다.우리는 여기서 섬유상 박테리오파지, 그 중에서도 M13 박테리오파지를 기반으로 간단한 풀링(Pulling) 과정을 거쳐 주기적인 나노 구조를 형성 할 수 있었다. 풀링(Pulling) 속도, 박테리오파지 농도 등의 조절을 통해 나노 구조의 주기성을 변화시켜 다양한 구조색을 얻을 수 있었고, 이러한 나노 구조를 온도를 조절할 수 있는 기판위에 형성하여 온도에 따른 색 변화를 관찰 할 수 있었다. 우리는 박테리오파지에 기반을 둔 컬러 디스플레이가 주목받는 차세대 디스플레이로 발전 할 수 있을 것이라 기대하고 있다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-451**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Preparation of carbon nanotube supported SnO_2 with enhanced dye degrading activity

이성규 최현철*

전남대학교 화학과

Organic dyes are widely used in various fields. However, dye-bearing effluents cause environmental problems because most of industrial dyes are considered to be one of the harmful and poisonous compounds. Therefore, semiconductor-assisted photocatalysis has recently emerged as an efficient method for degrading harmful dyes into environmentally compatible products. As one of the most important semiconductor oxides, tin oxide (SnO_2) has been studied using for photocatalyst. In this work, tin dioxide–carbon nanotube (SnO_2-CNT) nanocomposites were prepared successfully, by deposition of SnO_2 nanoparticles onto surface modificated CNTs. The obtained sample was characterized by transmission electron microscopy (TEM), powder X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The photocatalytic activities of the SnO_2–CNT nanocomposites were evaluated based on the photodegradation of methylene blue (MB) and methyl orange(MO). A plausible photocatalytic mechanism is discussed

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-452**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Nitrogen-rich carbon derived from melamine-based porous polymer for efficient carbon dioxide capture

Adeela 박수진*

인하대학교 화학과

Organic compounds including covalent organic framework, covalent organic polymers and metal─organic frameworks is one of the rapid growing fields of interest from few decades with the introduction of most efficient and economical material for CO_2 capture and storage. Here in, porous organic polymer based on melamine (MBPP) was prepared by single step polycondensation of isophthalaldehyde and 2,4,6-triamino-1,3,5-triazine via Schiff base chemistry. The synthesized polymer was subjected to pyrolysis at 800^{o}C to produce nitrogen rich porous carbon (NRC). CO_2 measurements were performed on designed materials and optimum uptake was achieved to be 128.37 mg/g (2.91 mmol/g) at 273k and 1 bar pressure with the specific surface area of 445 m^2/g. The excellent capturing ability and selective adsorption of CO_2 over N_2 was attributed to the presence of basic nitrogen ring in polymer chain and microporous texture of as prepared materials.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-453**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Photocatalytic activity of Fe_2O_3-CNT for the degradation of congo red

이성규 최현철*

전남대학교 화학과

Recently, there have been great interest in metal oxides decorated CNTs for applications in heterogeneous catalysts, fuel cells and biosensors. The most appealing metal oxide is a ferric oxide(Fe_2O_3) because of low cost, non-toxicity, outstanding stability, great surface area, oxide is a wide bandgap semiconductor (Eg=2.2 eV) with important technological applications in several fields. When ferric oxide(Fe_2O_3) particles are illuminated with which they degrade organic molecules absorbed on the surface of a photo catalysts. In this work ferric oxide – carbon nanotube (Fe_2O_3-CNT) nanocomposites were synthesized by a sol-gel method. The obtained photocatalyst was characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The photocatalytic activities of the prepared Fe_2O_3-CNT catalysts were evaluated under UV irradiation of CR degradation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-454**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Facile synthesis of amide-linked polymers and nitrogen doped carbon materials as potential sorbents for CO_2 Capture

Adeela 박수진*

인하대학교 화학과

Porous organic polymers possessing CO_2-philic moiety gained much attention for their efficient CO_2 adsorption capability. Based on the combination of purely organic rigid and contorted macromolecular structures with low skeletal density, amide-linked organic framework polymers, have been synthesized using cost-effective protocol. Polyamide chains were synthesized via low temperature condensation between 2,4,6-triamino-1,3,5-triazine and terephthaloyl chloride and isophthaloyl chloride to yield PA-1 and PA-2, respectively. The synthesized polymers were further carbonized at 600^{o}C to fabricate nitrogen containing carbon material. These as prepared materials were subjected to analyses including FTIR, XRD, TGA, FESEM, elemental analysis, XPS, specific surface area and pore size analysis and CO_2 adsorption measurements. The triazine ring with basic nitrogen atom and amide linkage in main chain are responsible for CO_2 capture.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-455**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Upconversion luminescence properties of tri-ions-doped $NaYF_4$ nanoparticle by NIR excitations

정종원 GerelkhuuZayakhuu 이용일*

창원대학교 화학과

Lanthanide ion(Ln^{3+})-doped up-conversion nanoparticles (UCNPs) are able to absorb NIR photons and convert such low energy excitations into shorter wavelength emissions. Utilizing long-lived, ladder-like energy levels of Ln^{3+}, the intensity of anti-Stoke's luminescence of UCNPs is orders of magnitude more potent compared with those of conventional synthetic dyes or quantum dots (QDs). Due to these unique properties, UCNPs have emerged as a new class of materials in a wide range of applications, such as bio-sensing, chemical sensing, in vivo imaging, drug delivery, photodynamic therapy and photo activation.Herein, $Nd^{3+}/Yb^{3+}/Er^{3+}(Tm^{3+})$ cascade sensitized tri-doped $NaYF_4$ UCNPs were prepared by solvo(hydro)thermal reaction method using autoclave system. This study reports the UC luminescence characteristics of UCNPs which were synthesis at various activator/sensitizer ions concentration ratio. In additions, the UC luminescence spectra under different excitation wavelengths were studied. The annealed temperature dependence of crystalline structures, surface morphologies and phase transitions of prepared material was investigated by using X-ray diffraction (XRD), scanning electron microscopy (SEM), and photoluminescence (PL).

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발표코드: **MAT.P-456**
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Synthesis and Optical Properties of Silver and Zinc Oxide Cationic Polyvinylpyrrolidone Nanocomposites

이승하 **ABDELAAL ALI** 이용일*

창원대학교 화학과

Polyvinylpyrrolidone is highly soluble in water and many non-aqueous solvents. And also PVP is easy to chemically modify. A cationic polyvinylpyrrolidone was synthesized by modification of polyvinylpyrrolidone, with 4-dimethylaminobenzaldehyde via aldol condensation reaction in basic media. Silver nanoparticles were prepared using reduction method by sodium citrate as reducing agent. The nanostructure of the synthesized cationic PVP with silver nanoparticles was prepared by self-assembling technique and investigated using UV and SEM techniques. The synthesized cationic PVP shows the ability to assemble on silver nanoparticles and form stable nanostructure with it. Zinc oxide nanoparticles capped cationic PVP was prepared by the sol-gel method and characterized using FTIR and SEM. The optical properties of the prepared nanocomposites were investigated by measuring the fluorescence and absorption spectra. The capping of ZnO nanoparticles with Cationic PVP led to surface passivation which increase the fluorescence and absorption compared to ZnO nanoparticles without polymer. This improvement of the optical properties is advantageous to the practical usage of ZnO nanocomposite such as bioimaging.

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Influence of Ag on thermal and electrical conductivity of epoxy composites in the presence of graphite and Copper

임윤지 박수진*

인하대학교 화학과

This study investigates the thermal and electrical conductivity of epoxy composites contacting hybrid fillers which are expanded graphite (EG), graphite (G), and copper powder (Cu). To enhance thermal conductivity of epoxy resin, EG were electrolessly Ag-plated (Ag-EG). Ag-EG. G and Cu are incorporated into the epoxy resin to form hybrid composites (Ag-EG/G/Cu). Ag-EG surfaces were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS). Thermal conductivity of Ag-EG/G/Cu composites was tested using a laser flash analysis (LFA). The electrical conductivity of the composites was tested using a four-point probe volume resistivity tester. From the results, it was found that the thermal conductivity of the composites was enhanced by addition of AG-EG/G/Cu hybrid fillers. In particular, the Ag-EG/G/Cu sample showed more than 755% enhancement of the thermal conductivity compared to the epoxy sample.

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Preparation and characterization of pitches from fluidized catalytic cracking-decant oils

임윤지 박수진*

인하대학교 화학과

To synthesize pitches, fluidized catalytic cracking-decant oils (FCC-DO) was heat treated according to treatment temperature and time. The pitches were characterized by measuring their elemental composition, chemical structure of components, molecular weight distribution, and softening point. The elemental composition and chemical structure was analyzed by element analyze (EA) and Fourier transform infrared (FT-IR). The molecular weight distribution was analyzed by matrix associated laser desorption ionization - time of flight mass spectrometry (MALDI-TOF). The FT-IR spectra demonstrated that the intensities of the aromatic C–H bonds at 1600 and 3030 cm-1 of the pitches significantly increased and the intensity of the stretching vibration of the C–H bond at 2920 cm-1 decreased with an increase in heat treatment time.

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Influence of Oxyfluorination on Geometrical Pull-out Behaviors of Carbon Fibers-reinforced Epoxy Matrix Composites

임윤지 박수진*

인하대학교 화학과

: In this study, the influence of oxyfluorination at different temperatures on the interfacial shear strength (IFSS) of carbon fiber/epoxy composites was investigated. The surface properties of the oxyfluorinated carbon fibers were studied through the measurement of XPS and SEM. A single fiber pull-out test was executed to investigate the basic characteristics of the single carbon fiber/matrix interface. Based on Greszczuk's geometrical model, the debonding force for pull-out of the fiber from the resins was discussed. It was shown that the surface functional groups containing oxygen on the oxyfluorinated carbon fibers exert strong effects on the surface energetics of fibers. Moreover, the formation of CFx physical bonding of the carbon fibers with fluorine increases the surface polarity of the fibers, resulting in increased IFSS of the composites, due to the improvement of interfacial adhesion between fibers and matrix resin.

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Intracellular Delivery of a Protein Using Cubic MSN with Ultralarge Pores

김기정 허성*

한국외국어대학교 화학과

Porous inorganic nanoparticles are emerging as efficient delivery nanocarriers for small molecules and drugs. To expand the range of cargos from small molecules to large native functional proteins, cubic mesoporous silica nanoparticles (cMSNs) with Pm3n pore symmetry were prepared. The as-prepared cMSNs were subsequently etched with a $Ca(NO_3)_2$ solution to expand their mesopores. The original mesopores with a pore dimension of 2.41 nm partially collapsed and combined into ultra-large mesopores with an average pore diameter of 13.89 nm without perturbing the original cubic symmetry of the remaining mesopores. Various techniques including powder X-ray diffraction, transmission electron microscopy, and electron tomography identified the unique three-dimensional structure of pore-enlarged cMSN (Ca-cMSN). The intracellular delivery of functional protein such as Cre recombinase into human TE671 cells was realized by using R8-Ca-cMSN as a native protein delivery synthetic nanocarrier.

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Modulation of the phase transition of VO_2 film by the W doping

이명순 김 돈*

부경대학교 화학과

The phase transition of the functional VO_2 film could be adjusted to near room temperature by the doping of W^{6+}(0, 0.43, 0.9, 1.8 and 3.6 atomic mol % of W). The films were prepared by the one step heating process, 30 min at 520°C, of the spin coated precursor mixture solution (VO_3NH_4 +$C_2H_2O_4$ + PVP + H_2O + ammonium tungstate) on sapphire substrate. The clear and sharp metal to insulator transition (MIT) of the VO_2 phase transition at ~ 340 K became unclear continuous transition along with the doping level of W atom. The hysteresis gap of the optical transition between cooling and heating cycle reduced from 25 K to 5 K by the addition of the W atom. Even the shape of the transition is changed, the starting point of the transition was constant value, ~ 340 K. These suggest the doped impurities induce the transition. Optical, electrical and thermal transition of the film will be discussed.

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Sensor applications of metal nanoparticles decorated on MWCNT (MNPs-MWCNT, M=Au, Pt)

이명순 김 돈*

부경대학교 화학과

This work describes a simple synthesis method of metal nanoparticles attached to multi-walled carbon nanotubes (MNPs-MWCNT, M=Au, Pt) by direct thermal decomposition and their applications as sensor. The direct thermal decomposition synthesis was carried out using metal precursor and could produced uniform MNPs (M=Au, Pt) on the surfaces of MWCNTs. MNPs-MWCNT (M=Au, Pt) were characterized by Raman, XRD and TEM and applied as field effect transistor sensor for carbohydrates detection and electrochemical sensor for neurotransmitters. The AuNPs-MWCNT FET sensor showed the high sensitivity (3.4 mM^{-1} for sucrose and 6.9 mM^{-1} for glucose) enough to diagnosis diabetes from a patient serum. The electrochemical sensor using PtNPs-MWCNT showed the excellent electrocatalytic response in the simultaneous determination of serotonin (5-hydroxytryptamine or 5-HT) and dopamine (DA) in presence of ascorbic acid. (DOL: 20 nmol $L^{-1}$for DA and 5 nmol L^{-1} for 5-HT)

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Structure and electrochemical properties of a new compound in potassium cobalt oxide as cathode material for rechargeable calcium ion battery

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Today, batteries have many applications such as power grids, solar power generation, transportation, medical and etc. Because multivalent cations, i.e., Ca^{2+}, Mg^{2+}, Al^{3+}, etc., are associated with more than one electron per ion, more energy can be stored in multivalent-ion batteries than those based on monovalent ions, such as lithium ion.In this work, a layered structure potassium cobalt oxide was prepared via a solid state method from potassium hydroxide and cobalt oxide at 600 ^{o}C under dry O_2. After near half amount of potassium were extracted by a charge process in calcium perchlorate electrolyte, and the electrode being washed, calcium ions were inserted to the electrode during a discharge process. The structural characterization, SEM and electrochemical properties will be reported.

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Synthesis and Characterization of Pyrene chromophores for Noncovalent Sidewall Functionalization of Carbon Nanotube Buckypapers

<u>최준</u>

한국생산기술연구원

Four pyrene derivatives were designed and synthesized in order to examine the noncovalent sidewall functionalization effect on the mechanical and electrical properties of multiwalled carbon nanotube buckypapers. The high-density carbon nanotube buckypapers were prepared by wet-laid process from homogeneously dispersed carbon nanotubes in water using a high-pressure homogenizer. The electrical conductivities of the buckypapers were increased dramatically after the noncovalent sidewall functionalization because of the enhanced charge transfer efficiency. Some of the functionalized carbon nanotube buckypapers also exhibited enhanced mechanical properties induced from the higher packing density and the tendency of alignment.

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Multiplexed biomolecule detection strategy using optokinetically encoded nanoparticles

김선기 남좌민*

서울대학교 화학부

Multiplexed real-time analysis on multiple interacting molecules and particles is needed to obtain valuable information in a complex medium, often found in chemical and biological systems. In particular, multiplexed profiling of microRNA (miRNA) in a reliable, quantitative manner is of great demand for the use of miRNA in cell biology, biosensing and clinical diagnostic applications. Here, we report a multiplexed miRNA detection strategy using optokinetically (OK) coded nanoprobes (NPs) that show distinct optical signals and dynamic behaviors on a supported lipid bilayer (SLB) (OK-NLB assay). Metal NPs with three distinct dark-field light scattering signals [red (R), green (G) and blue (B)] and three different target miRNA half-complements were tethered to two dimensionally fluid SLB with mobile (M) or immobile (I) state. In situ single-particle monitoring and normalized RGB analysis of the optokinetically combinatorial assemblies between three M-NPs and three I-NPs with dark-field microscopy (DFM) allow for differentiating and quantifying 9 different miRNA targets in one sample. The OK-NP-based assay enables simultaneous detection of multiple miRNA targets in a highly quantitative, specific manner within 1 hour, and can be potentially used for diagnosis of different cancer types.

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Synthesis of niobium diselenide nanosheets and their energy storage application

우준혁 백승민*

경북대학교 화학과

A class of materials known as transition metal dichalcogenides (TMDs) have two-dimensional structure with a wide range of unique mechanical, electrical, and chemical properties. The niobium diselenide ($NbSe_2$) nanosheets were synthesized in the liquid phase via solvent exfoliation using an interaction with the proper solvent. According to XRD patterns of $NbSe_2$ nanosheets, the intensity of (001) peak has been considerably decreased, showing that the $NbSe_2$ bulk was exfoliated into the nanosheets. Moreover, we confirmed the morphology of $NbSe_2$ nanosheets from the transmission/scanning electron microscopy studies. Also, electrochemical charge/discharge tests have been performed to investigate their applicability in rechargeable sodium ion battery.

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The role of additive to improve efficiency of binary organic photovolotaics

김정아 남민우 고두현*

경희대학교 응용화학과

In organic photovoltaics(OPV), the ratio of additive gives rise to a significant impact on efficiency. To find the additives and their proportions that can yield optimum efficiency, we fabricate OSCs that blended poly[[2,6′-4,8-di(5-ethylhexylthienyl)benzo[1,2-b;3,3-b] dithiophene][3-fluoro-2[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl]](PTB7-Th) and ITIC-Th as active layer with two different additives, 1,8-diiodooctane (DIO) and 1-chloronaphthalene (CN). As a result, OSCs with DIO showed higher efficiency than those with CN.

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Preparation of Mesoporous Silica and Organosilicas in the Presence of Pentablock Copolymer Templates

최은지 박재서 김태연 조은범*

서울과학기술대학교 정밀화학과

We were prepared the mesoporous silicas using tetraethyl orthosilicate (TEOS), 1,2-bis(triethoxysilyl)ethane (BTEE) and 1,4-bis(triethoxysilyl)benzene (BTEB). The copolymer template used here was a pentablock copolymer template of poly(D,L-lactic acid-co-glycolic acid)-b-poly(ethylene oxide)-b-poly(propylene oxide)-b-poly(ethylene oxide)-b-poly(D,L-lactic acid-co-glycolic acid) (PLGA-PEO-PPO-PEO-PLGA). Pentablock polymers were synthesized with commercial Pluronic F68 $EO_{75}PO_{30}EO_{75}$ and Pluronic F108 $EO_{128}PO_{54}EO_{128}$. The mesoporous silica samples were obtained simply by sol-gel chemistry under acidic conditions. The synthesized mesoporous silicas showed both nanoparticles and core-shell structures. Especially, mesoporous ethanesilicas prepared with BTEE showed higher surface area over the 1000 m^2/g which is proved by nitrogen adsorption analyzer. Also, some of mesoporous silica and organosilicas showed higher pore diameters and larger wall thicknesses over 10 nm than those of typical mesoporous materials. Detailed structure and compositional analysis will be demonstrated in this presentation.

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Enhancement of quantum dot luminescence via coupling with whispering gallery mode

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경희대학교 응용화학과 [1]경희대학교 화학과 [2]경희대학교 응용과학대학 응용화학과

Many studies to enhance broadband light absorption rate have been attracting intense interests as a matter of improving optoelectronic devices performance, such as solar cells and photodetectors. Spectral conversion technologies via downshifting nanoparticles are applied to broaden optical absorption wave width. In the case of ultraviolet light absorption field, downshifting luminescence abilities of quantum dots (QD), as well as fluorescent dyes, are good methods to increase the light absorption rate. Traditionally, QD in flim form is used as a downshifting material, but it has a disadvantage such that the efficiency improvement is limited. In this study, by using Layer-by-Layer(LBL) technique, we have QD adsorbed on the surface of optical nano-spherical cavity resonators, known as whispering-gallery mode(WGM) in order to amplify absorption and emission of light simultaneously. This QD-WGM bead's light trapping capability in wide-length frequencies can be widely used in solar cells, photodetectors, or nano-lasing applications.

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Facile metal transfer method to fabricate nanosize metal structure

김병훈 고두현*

경희대학교 응용화학과

Metal structures show large surface plasmon resonance effect due to its abundant free electrons. In order to generate surface plasmon effects at the visible range, subwavelength metal nanostructures should be provided. However, the conventional methods, such as photolithography or nanosphere lithography method, could only produce limited form of the metal nanostructures. In this study, we developed periodic metal nanostructure transfer method which could be adapted to the various substrates such as SiO2 and polymer layer. These structures have been further employed as metal mask due to its high etching selectivity. With metal nanostructure transfer method, we not only optimized localized surface plasmon resonance at the visible range but also achieved nanopatterned substrate via RIE etching process.

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발표분야: 재료화학
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Quaternary organic photovoltaics with High efficiency and long-term stability

유재홍 남민우[1] 고두현[1,*]

경희대학교 화학과 [1]경희대학교 응용화학과

The commercialization of organic photovoltaics (OPVs) must have attaining long-term morphological stability of the bulk heterojunction (BHJ) layer. Here we demonstrate the use of quaternary BHJs (q-BHJs) composed of two conjugated polymer donors and two fullerene acceptors as a novel platform to produce high-efficiency and long-term durable OPVs. A q-BHJ OPV (q-OPV) with experimentally optimized composition exhibits an enhanced efficiency and extended operational lifetime than does the binary reference OPV.

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발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

High-density Cisplatin-encapsulated Polymeric Nanostructures with Robust Stability and pH-sensitive Cargo-releasing Properties

이상민

가톨릭대학교 화학과

Over the past decades, biocompatible polymers have been proposed as a delivery platform for the improved aqueous solubility and reduced off-target toxicity for small-molecule drugs, allowing for the selected delivery to the disease sites. Although such delivery systems have been demonstrated to possess great potential to decrease the toxic side effects often associated with conventional chemotherapy, successes have been limited due in part to the limited colloidal stability and specific triggers to release the encapsulated drug molecules under predefined biochemical condition. To overcome these challenges, we have developed two strategies based on the chemically modified natural polysaccharides such as chitosan and artificial synthetic block-copolymers for polymeric excipients to encapsulate cisplatin pharmacophore (Pt^{II}) as a model drug. For stability enhancement and inorganic drug-conjugation, native chitosan was modified with small poly(ethylene glycol) and malonic acid, which was then subjected to bind the aqua derivatives of Pt^{II} species. As a synthetic polymer-based platform, a series of poly(ethylene glycol)-*b*-poly(acrylic acid) copolymers have been synthesized via nitroxide-mediated radical polymerization with chemically modified alkoxyamine initiator, which was then employed to incorporate the chemotherapeutic Pt^{II} compounds. Both approaches lead to the formation of self-assembled nanoscale structures in aqueous solution, which possess the grafted polymer chains cross-linked via Pt^{II}-coordination and hydrophobic interactions, allowing for the enhanced colloidal stability and pH-sensitive reversible release of Pt^{II} species. The physicochemical properties of the resulting materials will be demonstrated.

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장소: 일산 KINTEX
발표코드: **MAT.P-473**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

세리아 폐 파우더를 이용한 고효율 유막제거제의 개발

배지현 김민기 김운중*

한남대학교 화학과

자동차용 유리에 유막물질이 다량 흡착시, 빛 굴절율의 차이로 운전자의 시야가 정확히 확보되지 않아 사고위험이 매우 높게 된다. 따라서 금속, 유리등의 표면에 있는 유막을 제거하기 위해 실리카, 세리아(CeO2), 알루미나 입자 등이 사용된다. 이러한 다양한 유막제거제들 중 실리카 겔과 알루미나 백은 소재가 hard 하기 때문에 스크래치가 발생하는 경우가 많고, 또한 유막제거가 잘 되지 않아 유막제거가 어렵고 시간이 많이 걸리는 문제가 있다. 그러나 세리아는 소재가 soft 하기 때문에 상대적으로 스크래치 발생 위험이 적다. 하지만 큰 세리아 입자의 응집체가 많으면 스크래치가 발생하기 때문에 분산이 매우 중요하다. 또한 세리아 자체의 밀도가 높아 장기간 보관 시 세리아 입자들이 침전되어 재분산이 어려운 문제점이 있다. 따라서 본 연구는 세리아의 분산안정성을 높이고 장기간 보관에서도 침전이 발생하지 않는 친환경 유막제거제의 개발을 목적으로 연구를 진행하였다. 안정성을 높이기 위해 세리아 파우더에 -COOH 관능기 특성의 잔탄검을 사용하였고 테스트는 시판중인 타사의 유막제거제들을 가지고 차량에 테스트를 진행하였다. 세리아 파우더와 잔탄검의 수소결합으로 네트워크를 형성하여 점도를 높여 밀도가 높은 물질의 침강을 방지하여 분산안정성을 높일 수 있었다. 유막제거제 테스트 결과 시판중인 타사의 유막제거제와 성능 비교시 항목별 우수성이 높은 것을 확인하였다.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-474**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The improvement of power conversion efficiency by anti-reflection effect for CIGS solar cell

이경희 박상필[1] 고두현*

경희대학교 응용화학과 [1]경희대학교 화학과

Copper Indium Gallium Selenide (CIGS) solar cell is being studied actively as a renewable energy source. The conventional CIGS solar cell with thin photoactive layer suffers insufficient absorption due to reflection of incident light, thereby resulting in relatively low power conversion efficiency. In our study, we explored optical haze pattern simply prepared by the thermal evaporation and subsequent DI boiling process. The haze film was replicated the prepared pattern by introducing imprint method. The haze film improves CIGS device performance by elongating optical path length of incident light.

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장소: 일산 KINTEX
발표코드: **MAT.P-475**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Structural Formation Mechanism of Porous Carbon Nanosheets Synthesized by Pyrolysis of Organic salts

윤하나

한국에너지기술연구원 분리변환소재연구실

Porous carbon nanosheets have attracted much attention because of their unique properties including short diffusion lengths and structural stability. They show promise in as electrode materials for energy storage, water purification agents, and catalytic supports. In recent years, porous carbon nanosheets synthesized by pyrolysis of organic salts have been reported. but their structural formation mechanism has been remained unclear. In this study, the formation mechanism of porous carbon nanosheets was thoughtfully studied by SEM, XRD, in-situ TEM, and TGA. The role of the intermediate products in the formation of porous carbon nanosheets was elucidated.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-476**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Heteroatom-containing functionalities in N-doped reduced graphene oxide for oxygen reduction reaction electrocatalyst

신윤석 박성진*

인하대학교 화학과

Amounts of N and O atoms in N-doped graphene oxide are important to understand why N-doped graphene-based materials show good performance as metal-free electrocatalysts for oxygen reduction reaction(ORR). In this work, we prepared ammonia-reduced graphene oxide(A-rG-O) using a solution process. A-rG-O samples thermally treated at high temperatures (300-700°C) for investigating between ORR performances of A-rG-O and the chemical structure.

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발표분야: 재료화학
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Color filters of ZnS Nanocavity structure without angle-dependence

조봉현 안태규[1,*]

성균관대학교 에너지과학 [1]성균관대학교 에너지과학과

In optical color filter system, generation of color pixels beyond the diffraction limit is a key aspect. Nowadays, large-scale nanofabrication techniques, such as nanoimprint lithography, roll-to-roll processing, colloidal self-assembly, and laser interference lithography, are widely utilized for color printing with sub-diffraction resolution. However, there are huddles in limiting optical resonances at the same wavelength over a wide angular range and in simultaneous creation of full colors in a pixel unit. To compensate angular-dependence, we used ZnS nanocomposites with high refractive index materials, which is reported to relieve the angular dependence. Herein we presented an angle invariant structural color-generation, based on ZnS patterned nanocavity on a flexible substrate. The nanocavity pattern structure has been fabricated over a large area by nanoimprint lithography, and revealed consistent performance over a wide angle of incidence up to 60°. In addition, the transmitted colors of the proposed structure of triple layers, can be tuned easily by changing the width of nano-gratings. Thus we enabled the creation of individual RGB colors in a pixel unit via a simple one-step approach. We believe that the presented nanocavity could provide a new aspect for achieving improved efficiency and desired optical functionality, thereby it will pave a way to achieve high performance structural color filters with addition applications including anti-counterfeit tag, imaging sensors, and colored e-paper displays.

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장소: 일산 KINTEX
발표코드: **MAT.P-478**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

An Efficient Role of RuO_2 Nanosheet as an Additive for Exploring High Performance Electrocatalysts

권남희 황성주*

이화여자대학교 화학·나노과학과

High performance electrocatalysts for oxygen evolution reaction (OER) can be synthesized by the hybridization between exfoliated layered double hydroxide (LDH) and highly conductive RuO_2 nanosheets. Mesoporous LDH—RuO_2 nanocomposites are synthesized by the electrostatically-driven self-assembling between negatively-charged RuO_2 nanosheet and positively-charged LDH nanosheet. The coupling with metallic RuO_2 nanosheet provides a quite effective way to improve oxygen evolution ability of LDH with a considerable drop of overpotential even similar with Ir/C. Compared with the mechanically mixing of LDH and RuO_2, LDH—RuO_2 composite shows much higher performance. Such a huge potential drop is originated from the increased electrochemically active surface area and active charge transfer. This efficient additive can be applied not only to a specific LDH but also to other LDH. The present results underscore that exfoliated RuO_2 nanosheet can be used as an effective additive for improving the electrocatalytic activity of LDH materials.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-479**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Realization of green and amber emissive AIZS/ZnS QD-LEDs

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In this study, we fabricated green and amber emissive AIZS/ZnS quantum dot light-emitting diodes (QD-LEDs). For facturing these two color of QLEDs, we synthesized green and amber AIZS/ZnS quantum dots by preparing core-forming, alloying, and shelling process at different temperatures. These QDs show broad band spectra (FWHM > 80nm) and have PLQYs of 41, 52%, respectively. Layers of QLED are composed of a PEDOT:PSS hole injection layer (HIL), a poly(9-vinylcarbazole) hole transport layer (HTL), a QD emitting layer (EML) and a ZnO nanoparticle electron transport layer (ETL). The devices that we fabricated have maximum luminance values of 999, 498 cd/m^2, and 1.12, 0.36 cd/A in current efficiency (CE) and 0.39, 0.25% in external quantum efficiency (EQE), respectively. Although EL performances are inferior to other Cd-based or CIS-containing devices, these green and amber emissive AIZS/ZnS QD-LEDs have much possibility for improvement in the near future.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-480**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of $CsPbX_3$ (X=Br, I, Cl) Inorganic perovskite Quantum Dot-based multi-package white down-converted LEDs

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국민대학교 화학과 [1]국민대학교 생명나노화학과

In this study, we synthesized the $CsPbX_3$(X=Br, I, Cl) inorganic perovskite quantum dots and fabricated multi-colored monochromatic down converted (DC) light emitting diode (LED). $CsPbX_3$ inorganic perovskite were synthesized via a colloidal hot injection method, their emission wavelength and Quantum yields (QY) can be tuned from 485nm to 640nm and from 50% to 85%. $CsPbX_3$ inorganic perovskite QD-based multi-colored monochromatic DC-LEDs were fabricated using InGaN blue LED chip, and long-wavelength pass dichroic filter (LPDF) which can pass the long wavelength and reflect the short wavelength. We fabricated the six color multi-package white DC-LEDs using Cyan, Green, Yellowish green, Orange, and Red colored monochromatic DC-LED and a InGaN blue LED and comparison of their optical properties of six-package white DC-LEDs compared using TM-30 color standard which indicates the correct evaluations of the color rendition. Additionally, we found the circadian prospective for the benefit to human health through the spectral power distributions such as color fidelity index (CFI) and color gamut index (CGI).

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-481**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of Low-temperature-sintered Phosphor-in-Glass to realize the white-LED package

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We dispersed YAG:Ce^{3+} phosphor with Sn-P-F based glass frit as light emitting diode (LED) inorganic encapsulant. We can obtain the phosphor in glass (PiG) based down-converted white LED (DC-WLED) with 210 ~ 250 ℃ low sintering temperature which can decrease the thermal defect of commercial phosphor. We realized these fabricated yellow emissive PiGs to package the cup-type white LEDs. These PiGs are expected to prevent the Sn-P-F based glass encapsulant from turning yellowing, causing the decrease of luminous efficacy (LE). The white LED realized the luminous efficacy of 110 lm/W (EQE = 0.303), respectively, at ~ 4500 K. Furthermore, it shows high temperature resistance in comparison of commercial silicone resin in temperature dependence test. The photoluminescence properties of phosphor were measured using Xe lamp and a spectrophotometer. The images of PiG based WLED were obtained by scanning electron microscopy (SEM). The PiG based WLED were measured using electroluminescence (EL) in an integrated sphere with applied current of 50 mA to 700 mA.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-482**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

New Organic Hole-Transporting Materials in Perovskite Solar Cells

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Organic inorganic halide perovskite shows great potential for photovoltaic applications due to long charge diffusion length, appropriate bad gap, solution processability, very low material costs, and high absorption coefficient,. During the last five years, the power conversion efficiency (PCE) of the perovskite solar cell (PSC) has been enhanced from 3.8% to 20%. The issues of the degradation of perovskite should be urgently addressed to achieve good reproducibility and long lifetimes for PSC. All PSC achievements from the laboratory can be transferred to front industries and outdoor applications, if the stability issue is overcome. Hole-transporting materials (HTMs) are now an integral part of PSCs. Both organic and inorganic HTMs have found application in PSCs. However, inorganic HTMs are hampered by the limited choice of materials and the relatively low PCE of the solar cells based on them. In this regards, we improved the stability of the PSC as well as the power conversion efficiency by optimizing the hole transport layer. One of advance has been accomplished by replacement of the liquid electrolytes by solid-state HTMs, which not only improves the power conversion efficiency (PCE) but also enhances the cell stability. We fabricated PSC devices with two new organic hole transport materials on the structure ITO/HTM/Perovskite/PCBM/ZnO/Al. A HTM material shows a better performance than commercial hole transport material PEDOT, with Jsc=19, PCE=16.87. Another HTM shows a comparable performance as PEDOT, with Jsc=17.49, PCE=14.35.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-483**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of Highly Efficient Green-Emitting Zn-Ag-In-S/Zn-In-S/ZnS Quantum Dots Using an Exothermic Reaction

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국민대학교 화학과 [1]국민대학교 생명나노화학과

In this study, we synthesized highly efficient green Zn-Ag-In-S/Zn-In-S/ZnS alloy-core/inner-shell/outer shell quantum dots (QDs) using a multistep hot injection method. This process is through a five sequential steps: Ag-In-S core growth, a two-step alloying/inner-shelling process by injecting the Zn-In-S source, and a two-step outer ZnS shelling process. To optimize photoluminescence quantum yield (PLQY) of QDs, we changed the concentration of zinc acetate dihydrate precursor for outer shelling. We confirmed that when ZAIS/ZIS/ZnS QD is synthesized with a high concentration of zinc acetate dihydrate, the PLQY increases because a strong exothermic reaction takes place during formation of ZIS inner-shell. To confirm the synthesis of highly efficient green-emitting Zn-Ag-In-S/Zn-In-S/ZnS, XRD, Raman, XPS, and TEM were utilized by analyzing the obtained QDs. The synthesized green ZAIS/ZIS/ZnS QDs reached a PLQY as high as 87% at a wavelength of 501 nm, which is the highest recorded value for green AIS-based QDs.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-484**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Synthesis of Nanocrystalline Vanadium Nitride and Its Application of Energy Storage System

박용진 김재겸 강경모 이하은 김승주[1,*]

아주대학교 에너지시스템학과 [1]아주대학교 에너지시스템학부

Transition metal nitrides are promising candidates for anode in lithium ion battery because they undergo the electrochemical conversion reaction with lithium and have great electrical conductivity. Herein, nanocrystalline vanadium nitride was synthesized via a metathesis reaction of Li_3N and VCl_3. X-ray diffractometer and scanning electron microscope were performed to confirm the crystal and micro structure. Nanocrystalline vanadium nitride delivers a capacity of 180 mAh g^{-1}, which is comparable to the reaction of around half lithium per VN unit upon charge-discharge cycling test. Additionally, cyclic voltammetry measurement was also performed. Nanocrystalline vanadium nitride gives rise to a series of reversible redox reactions and deliver an impressive specific capacitance for supercapacitor.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-485**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Enhancement of the CO_2 Adsorptivity of Metal Oxide via *In-Situ* Formation of Metal Sulfide Domain

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이화여자대학교 화학나노과학과 [1]이화여자대학교 화학·나노과학과

We are successful in preparing novel metal oxide-metal sulfide nanocomposites showing superior CO_2 adsorptivity. The heat-treatment of Mg-Al-layered double hydroxide (LDH) under sulfur-containing atmosphere yields sulfur-doped layered double oxide (LDO) of $MgO/MgAl_2O_4$. Although sulfur substitution has negligible influence on the crystal morphology of LDO, the incorporation of Mg-S bond is effective in remarkably improving its CO_2 adsorptivity. The observed improvement of CO_2 adsorption activity can be attributed to the enhancement of the bond ionicity of (Mg-O) via the competition with adjacent covalent (Mg-S) bond. The present study clearly demonstrates that the fine-tuning of the bonding character of basic metal oxide via sulfur substitution provides a universal and efficient way to optimize its CO_2 adsorbent functionality.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-486**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Improvement of Na Ion Electrode Performance of TiO_2(B) upon Composite Formation with Conductive TiS_2

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이화여자대학교 화학·나노과학과 [1]한국기초과학지원연구원 서울서부센터

The composite formation with conductive metal sulfide domain has advantageous effect on the Na-ion electrode functionality of metal oxide. In this research, we synthesized 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, clearly demonstrating 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 composite formation of semiconducting metal oxide and metal sulfide in exploring new efficient NIB electrode materials.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-487**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

III-V Quantum Dots GaAs, InGaAs and ZnSe shellwith Colloidal Method

서해운 권오훈[1] 안소연[1] 박수웅[1] 노재영[1] 김상욱[2,*]

아주대학교 분자기술학과 [1]아주대학교 분자과학기술학과 [2]아주대학교 응용생명화학공학부

As well-known GaAs is an important semiconductor that has attracted significant attention because of its use in solar cells and optoelectronics. It has a bandgap of 1.42 eV and a chalcopyrite crystal structure. GaAs Bohr exciton radius is 10 nm, also shows quantum confinement effects. Than the particle size decreases below the leading to visible light absorption and emission. GaAs based CQD, which are hard to obtain by the chemical synthetic method. But it can be prepared successfully using the acetylacetonate complex of indium and gallium as cationic precursors. We control the indium contents, and the photoluminescence emission is tuned from orange to deep red.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-488**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Hybridization of Metal-Organic-Framework with Layered Double Hydroxide Nanosheet to Enhance Its Water Adsorptivity

Haslinda binti Mohd Sidek 조윤경[1] 황성주[2,*]

이화여자대학교 화학·나노과학 [1]이화여자대학교 화학나노과학과 [2]이화여자대학교 화학·나노과학과

The hybridization of metal-organic-framework (MOF) with exfoliated layered double hydroxide (LDH) nanosheet is effective in improving its water adsorption functionality and in enhancing its hydrostability. The nanoscale mixing of MOF and LDH components can be achieved by the electrostatically-derived self-assembly between the opposite surface charge of anionic copper-benzene tricarboxylate (Cu-BTC) MOF nanocrystal and cationic Mg-Al-LDH nanosheet. The resulting nanohybrids exhibit the uniform anchoring of small-sized Cu-BTC nanoparticle (~5-10 nm) on the surface of Mg-Al-LDH nanosheet. The surface area of the resulting nanohybrid with optimal LDH content is greater than that of the pristine Cu-BTC, which is attributable to the depression of the self-aggregation of MOF nanocrystals and to the formation of the mesoporous stacking structure of LDH nanosheets, respectively. Of prime importance is that both the water adsorption ability and hydrostability of Cu-BTC become remarkably improved upon hybridization with LDH nanosheet. The present study clearly demonstrates the effectiveness of the exfoliated LDH nanosheet as a hybridization matrix for synthesizing novel efficient MOF-based hybrid water adsorbents.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-489**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrochemistry of Graphitic Carbon Nitride Synthesized from Various Precursors for Catalytic Effects

오정훈 박성진*

인하대학교 화학과

Graphitic carbon nitride (g-C_3N_4) synthesised by pyrolysis of dicyandiamide, melamine and urea precursors under varying reaction conditions (air and N_2) is subjected to electrochemical studies for the elucidation of the inherent catalytic efficiency of the material. Contrary to popular belief, pristine g-C_3N_4 shows negligible, if any, enhancement in its electrochemical behaviour in this comprehensive study. Voltammetric analysis reveals g-C_3N_4 to display similar catalytic efficiency to the unmodified glassy carbon electrode surface on which the bulk material was deposited. This highlights the non-catalytic nature of the pristine material and challenges the feasibility of using g-C_3N_4 as a heterogeneous catalyst to deliver numerous promised applications.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-490**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Composite Hollow Nanostructures Composed of Carbon-coated Ti^{3+} Self-doped TiO_2-Reduced Graphene Oxide as an Efficient Electrocatalyst for Oxygen Reduction

boppella rami reddy 김동하[1,*]

이화여자대학교 화학나노 [1]이화여자대학교 화학나노과학과

Cost-effective durable and highly active electrode materials have become greatly desirable in the electrocatalytic oxygen reduction reaction (ORR), a crucial element in energy devices. In particular, the low intrinsic conductivity and poor reactivity of TiO_2 are believed to hinder an efficient applicability of this material as an ORR catalyst. Herein, we report for the first time an efficient one-step approach to synthesize conductive Ti^{3+} self-doped carbon-coated TiO_2 anchored on reduced graphene oxide (rGO) hollow nanospheres. A remarkable 11-fold improvement of the conductivity of TiO_2 with an optimized rGO(10%)/TiO_2 sample is herein reported. The rGO/TiO_2 hollow nanospheres unveiled comparable activity to that of a conventional Pt/C reference. Most importantly, improved stability and remarkable methanol tolerance were achieved. Results were attributed to a cooperative effect of the hybridization of TiO_2 with rGO, Ti3+ self-doping and the formation of a carbon-coating layer over the TiO_2 particles. The selected design for the morphology of this novel electrocatalyst was further confirmed to play a crucial role in providing an enhanced number of active sites for oxygen reduction. This new nanocomposite is believed to exhibit promising applicability in a wide range of research areas including energy storage and conversion, photocatalysis, and gas sensors.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-491**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Antimalarial drug-Zinc Basic salt Hybrid Durg ; Oral and Intravenous Administration Routes

김지영 최진호* **PIAOHUIYAN** 최고은

이화여자대학교 화학.나노과학과

Artesunate (AS) is the most widely used artemisinin derivative as an effective anti-malaria drug. However, AS shows a low oral bioavailability due to the poor aqueous solubility and instability in acidic solution. Therefore, we incorporated AS molecules into hydrophilic zinc hydroxide layers (ZBS), which was studied as a reservoir or carrier for fragile bioactive molecules, not only to increase aqueous solubility of AS but also to enhance its chemical stability under an acidic condition. According to the x-ray diffraction analysis, the basal spacing of ZBS-AS nanohybrid was determined to be 2.88nm, indicating that AS was successfully incorporated into ZBS layers, which was also confirmed by 1-D electron density mapping along the crystallographic c-axis and transmission electron microscopic analysis. The FT-infrared spectroscopic analysis revealed that AS molecules were deprotonated and electrostatically interacted with cationic zinc hydroxide sheets. From CHNS, TG and HPLC analyses, the content of AS encapsulated in ZBS vehicle could be estimated as ~46 wt%, and the chemical formula of thus prepared ZBS-AS nanohybrid was determined to be $Zn_5(OH)_8(C_{19}H_{28}O_8)_{1.1}(Cl)_{0.9}\cdot 3H_2O$. Furthermore, in order to enhance the dissolution property of AS in simulated intestinal condition, ZBS-AS nanohybrid was coated with enteric coating polymer, Eudragit® L100, (ZBS-AS-L100). Finally we have performed in-vivo pharmacokinetic study in rats via oral administration in order to compare absorption of AS of ZBS-AS-L100 nanohybrid with that of intact AS, and surprisingly, it was found that the former was ~6 times larger than the latter due to an enhanced solubility of AS thanks to the hybridization with hydrophilic ZBS. Therefore, ZBS-AS-L100 could be suggested as a promising drug delivery system for improving drug solubility and absorption. Additionally, we encapsulated AS molecules into layered double hydroxide (LDH) for intravenous injection, and then, systematically discussed on the AS release property in the simulated body fluid solution, which will be demonstrated in-detail in the presentation.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-492**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Enhanced Mechanical and Heat release rate Property of EVA Nanocomposites with Cationic and Anionic Clays

이지희 류현주 양재훈 최진호*

이화여자대학교 화학.나노과학과

2-dimensional compounds including cationic and anionic clays are a new class of inorganic fillers for improving thermal and mechanical properties of polymer. In this work, we synthesized ethylene vinyl acetate (EVA) copolymer nanocomposites containing cationic and anionic clays via solution blending method. Cationic and anionic clays were modified with hydrophobic surfactant via co-precipitation and ion-exchange method in order to increase the compatibility with hydrophobic EVA polymer matrix. The organically modified cationic and anionic clays were dispersed in toluene and blended with EVA solution to form EVA nanocomposites depending on the mixing ratio of organo-clays to EVA. According to the X-ray diffraction analysis, (00l) peaks corresponding to the organic clays were disappeared due to the exfoliation into individual sheets and their homogeneous dispersion in EVA matrix. The thermal stability of EVA nanocomposites were gradually improved by increasing the content of organo-clays. Mechanical properties such as elastic modulus and tensile strength of EVA nanocomposites were remarkably enhanced by increasing the amount of organo-cationic clay, because of the high dispersity of organo-clays in EVA matrix. EVA nanocomposites containing organo-clays showed the significantly reduced heat release rate (HRR) property, indicating the potential as promising flame retardant materials. These improvement could be attributed to the high dispersity of 2- dimensional clay nanosheets organo-clays in EVA matrix.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-493**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Mesoporous Geopolymers containing acidic sites with Enhanced Thermal and Hydrothermal Stability

PEIYIRONG 양재훈 최진호*

이화여자대학교 화학.나노과학과

Mesoporous silica is one of the most desirable materials in the catalytic and adsorption research fields due to their high surface area and uniformed porous structure. However, mesoporous silica is unstable under high temperature and hydrothermal conditions. And to overcome such disadvantages, many efforts for improving their thermal and hydrothermal stability have been carried out such as metal ions post-doping, such as metal ions post-doping, such as Al^{3+} and Fe^{3+} in the silica framework, and zeolite seeding to make the framework structures thick and highly crosslinked. Recently, we were very successful in enhancing thermal and hydrothermal stabilities of mesoporous silica simply by designing the mesoporous geopolymer from meta-kaolin. In brief, meta-kaolin and silicon precursors such as fumed silica or sodium silicate were dissolved in a strong alkaline solution with the pH ~14 to form a viscous solution, which was then mixed with 55 mM of cetyltrimethyl ammonium bromide solution, where the molar ratio of Si/Al was varied from 3 to 10. The solution pH was finally adjusted to 10.5 by adding HCl solution and hydrothermal treatment at 100^oC for 24 h. The resulting white precipitate was completely washed with water and dried and calcined at 550^oC for 6h. According to the XRD analysis, the synthesized mesoporous geopolymers were turned out to have the hexagonal type-pore structure similar to the MCM-41 mesoporous silica. From the N_2 adsorption-desorption isotherm analysis, specific surface area and pore volume of the mesoporous geopolymers were increased from 400 m^2/g to 650 m^2/g and from 0.5 cm^3/g to 0.75 cm^3/g, respectively, with increasing the Si/Al ratio from 3 to 10. The pore structure of geopolymer with Si/Al = 5 (SEG-41-5) remained unchanged up to 900^oC, while MCM-41 prepared via conventional method was stable up to only 800^oC but its porous structure was completely colapsed at 900^oC. Furthermore, under the hydrothermal condition at 100^oC, SEG-41-5 retained its mesoporous structure up to 7 days, while the pore structure of MCM-41 was completely decomposed after 2 days. This is purely

due to the fact that mesoporous geopolymer results in an improved thermal and hydrothermal stability compared to mesoporous silica.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-494**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

PLP-LDH Nanohybrid as mineral supplement for patients with type 2 diabetes mellitus

류현주 심서영[1] 최고은 최진호*

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학나노학과

Recently, layered double hydroxides (LDH) have been developed as inorganic nanovehicles for delivering therapeutic agents. In this work, LDH containing Mg^{2+}, Zn^{2+} and Cr^{3+}, which are deficient minerals to the type-2 diabetic patients, were developed as mineral supplement for the patients. Furthermore, Vitamin B_6 (pyridoxal-5-phosphate; PLP), involving in the mechanism of insulin action and in glucose metabolism, was also incorporated into the interlayer space of LDH by ion-exchange method. According to the X-ray diffraction (XRD) analysis for PLP-LDH nanohybrid, the basal spacing of LDH was expanded from 8.6 Å to 16.5 Å, indicating that the PLP molecules were successfully intercalated into the interlayer space of LDH. Fourier transform infrared (FT-IR) spectra also revealed that the PLP molecules were deprotonated and stabilized between the LDH layers through electrostatic interaction. The scanning electron microscopy (SEM) images showed that the PLP-LDH nanohybrid had a thin, plate-like morphology with a uniformed size (~ 100 nm). The photo-stability assay of PLP and PLP-LDH nanohybrid were carried out under UV light. The content of PLP in PLP-LDH nanohybrid at 180 min after light irradiation was retained more than 95 % of initial content, while that of pure PLP was decreased down to ~ 28 %. This is due to the fact that the PLP molecules are thermodynamically more stabilized in the interlayer space of LDH by electronic interaction even under UV irradiation condition. MTT assay with L929 mouse fibroblast cell-line, no signification cytotoxicity could be observed for PLP-LDH nanohybrid with a dosage less than 500 ug/mL. And therefore, we suggest that this PLP-LDH nanohybrid may have a potential application as the novel drug storage system.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-495**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Organic Nonvolatile Resistive Switching Memory

김재준 **Masaki Kawano***

Tokyo Institute of Technology, Japan

Among various memory devices, resistive random access memory (ReRAM) have emerged as a next generation nonvolatile memory device because of its high density integration, low power consumption, and simple architecture. Especially, the use of organic materials as an active layer provides many advantages including flexibility, low fabrication costs, and so on. Although a number of organic nonvolatile memory devices have been extensively explored, their switching mechanisms have been still ambiguous because of analytical difficulty. Indeed, the development of new material systems and investigating switching mechanisms are highly demanded to design high performance device. Here, we report bistable nonvolatile ReRAM based on 2,5,8-tri(4-pyridyl)1,3-diazaphenalete (TPDAP), which showed two stable resistance states which can be modulated by external electrical stimulation, high On/Off ratio, and stable retention and endurance. In addition, switching mechanism is proposed by in-/ex-situ spectroscopy measurement.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-496**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Cellular uptake of biocompatible yttrium incorporated layered double hydroxide for theranosis

엄새란 양재훈 최고은 최진호*

이화여자대학교 화학.나노과학과

Radiotherapeutic Yttrium-90 (90Y) has been known as a pure β-emitter with fewer environmental radiation restrictions, and therefore, considered to be suitable for the irradiation to large solid tumors because of its long residence time property. Recently, we have developed a novel radio-therapeutic system on the basis of 90Y incorporated layered double hydroxide (Y-LDH). According to our previous studies, LDH nanoparticles with ~100 nm in size, as a drug delivery carrier, could target not only the tumor tissues and but also the tumor cells due to superior intercelluar permeability, thanks to the clathrin mediated endocytosis and eventually dissolved slowly in the cytosol at the intracellular compartments such as late endosome and lysosome, where the pHs are rather acidic. Therefore, Y-LDH, [Mg2Al0.9Y0.1·(CO3)·nH2O], was designed and prepared by co-precipitation and successive hydrothermal treatment. From the X-ray diffraction (XRD), the crystal lattices of Y-LDH with a = 3.052 Å, c = 23.024 Å were slightly expanded along the crystallographic c-axis compared to those of pristine LDH with a = 3.047 Å, c = 22.908 Å, since the ionic radius of Y3+ is larger than that of Al3+. And the average particle size of Y-LDH was determined to be ~100 nm with a plate-like morphology, and they showed 2.5-fold higher cellular uptake efficiency as expected, in the mouse liver cancer cell compared with that in the normal cell, and very low cytotoxicity with no significant decrease in normal fibroblast cell proliferation at the concentration below 100 μg/mL. These results imply that the present Y-LDH can serve as a potential tool for the theranosis application.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-497**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Novel intercalation route to gallate incorporated layered double hydroxide nanohybrid : exfoliation and reassembling reaction

KANAKAPPAN MICKEL ANSY BENZIGAR ELSY DARLINE BENZI 이지희[1] 양재훈[1] 최진호[1,*]

이화여자대학교 화학나노과학과 [1]이화여자대학교 화학.나노과학과

Recently, layered double hydroxide (LDH) nanohybrids intercalated with bioactive molecules have attracted a great interests due to their biocompatibility and cancer targeting delivery property in nanomedicine. To understand the improved theranostic properties of LDH nanohybrids, it is required to synthesize LDH nanohybrids which are chemically and structurally well-defined. As for the encapsulation of bio active molecule, Gallic acid (GA), with antioxidant property was stabilized in the interlayer space of into well-defined LDH, exfoliation and reassembly reaction, which was realized by the conventional ion-exchange or co-precipitation reactions. At first, the nitrate-type Zn2Al-LDH, was synthesized via co-precipitation followed by the hydrothermal treatment at 80oC for 6h. Thus prepared Zn2Al-LDH was dispersed in formamide to form exfoliated LDH colloidal solution under nitrogen atmosphere. The exfoliated Zn2Al-LDH colloidal solution was reassembled to form GA intercalated LDH (GA-LDH) in the presence of GA in solution, where the pH was adjusted to pH 7 in order to deprotonate GA to form gallate anion. According to the XRD analysis, GA-LDH showed the well-developed (00l) diffraction peaks with a basal spacing of ~ 1.12 nm, which was larger than the of pristine Zn2Al-LDH (0.86 nm), indicating that gallate molecules were successfully incorporated into Zn2Al-LDH layers. From the FT-IR spectra it was found that gallic acid was completely deprotonated into gallate, and stabilized in between LDH lattices via electrostatic interaction. The content of GA in GA-LDH was determined to be ~ 23 wt% by the UV-vis spectroscopy and HPLC analyses. In vitro release test at pH 6.8 demonstrated that GA was sustainably released from GA-LDH nanohybrid up to 85% within 48h. The anti-oxidant property will also be systemically discussed on the basis of DPPH method. And therefore, the present reaction route to GA-LDH nanohybrid can be considered as one the cost-effective synthesis platforms for nanomedicine.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-498**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

TiO2/CdS-PANI nanostructure on FTO glass with the enhanced absorption andphotocatalytic performance for Hydrogen generation

김현 양비룡*

금오공과대학교 신소재공학과

TiO_2/CdS-PANI nanostructure has been demonstrated as the solar selective absorber coating for the first time. The effortless chemical methods and easily scalable techniques such as Hydrothermal, in-situ polymerization and spin coating were adopted for the fabrication of TiO_2 nanorods and TiO_2/CdS/PANI nanostructure for enhanced Hydrogen generation. The Electrochemical measurements were performed using a 1 kW xenon lamp (Newport) with its infrared wavelengths filtered out by water, and wavelengths below 420 nm removed by an optical filter, enabling measurements under visible light. The light irradiance, measured by a thermopile detector, was 100 mW/cm^2. A monochromator (74,000, Newport) was used to investigate the monochromatic responses (for IPCE, applied bias photon to current efficiency (ABPE), and band gap energy measurements) of samples.[1] the energy dispersive X-ray spectra and elemental mapping confirm the presence of the chosen elements in the nanostructure. Results indicate that the addition of the PANI nanoparticlesto the TiO_2/CdS/PANI nanostructure enhance the photocatalytic efficiency under natural sunlight irradiation. The optimized solar absorber coating of CdS-PANI nanostructure is highly promising for its selective optical properties

Figure 1: show potential energy level TiO2/CdS/polyaniline one-diensional nanohybrid, relative to the redox potential for water splitting

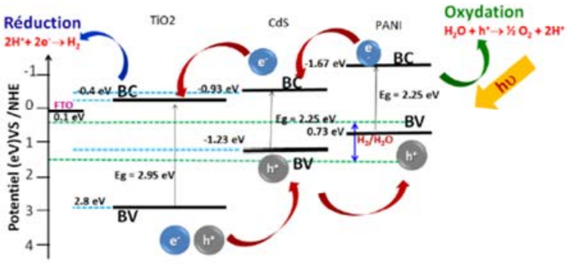
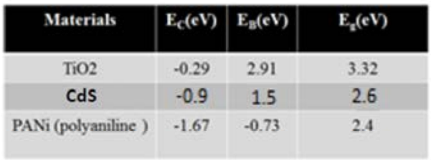


Table 1. Energy of band edge and gap



Materials	E_C(eV)	E_B(eV)	E_g(eV)
TiO2	-0.29	2.91	3.32
CdS	-0.9	1.5	2.6
PANi (polyaniline)	-1.67	-0.73	2.4

1. *Effect of seed layers on TiO2 nanorod growth on FTO for solar hydrogen generation. Hyun Kim, Bee Lyong Yang. International Journal of Hydrogen Energy 40(2015) 5807-5814.*

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-499**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

TiO2/In2S3-PANI nanostructure on FTO glass with the enhanced absorption andphotocatalytic performance for Hydrogen generation

김현 양비룡*

금오공과대학교 신소재공학과

TiO_2/In2S3-PANI nanostructure has been demonstrated as the solar selective absorber coating for the first time. The effortless chemical methods and easily scalable techniques such as Hydrothermal, in-situ polymerization and spin coating were adopted for the fabrication of TiO_2 nanorods and TiO_2/In2S3/PANI nanostructure for enhanced Hydrogen generation. The Electrochemical measurements were performed using a 1 kW xenon lamp (Newport) with its infrared wavelengths filtered out by water, and wavelengths below 420 nm removed by an optical filter, enabling measurements under visible light. The light irradiance, measured by a thermopile detector, was 100 mW/cm^2. A monochromator (74,000, Newport) was used to investigate the monochromatic responses (for IPCE, applied bias photon to current efficiency (ABPE), and band gap energy measurements) of samples.[1] the energy dispersive X-ray spectra and elemental mapping confirm the presence of the chosen elements in the nanostructure. Results indicate that the addition of the PANI nanoparticlesto the TiO_2/In2S3/PANI nanostructure enhance the photocatalytic efficiency under natural sunlight irradiation. The optimized solar absorber coating of In2S3-PANI nanostructure is highly promising for its selective optical properties

Figure 1: show potential energy level TiO2/In2S3/polyaniline one-diensional nanohybrid, relative to the redox potential for water splitting

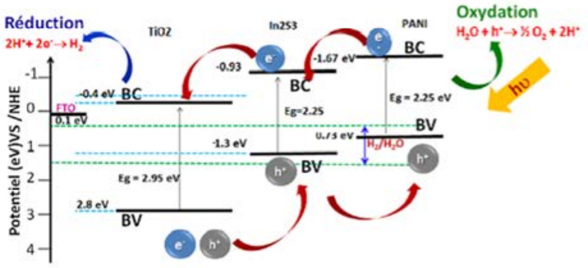
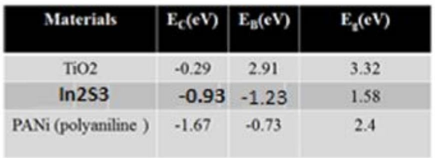


Table 1. Energy of band edge and gap



Materials	E_C(eV)	E_B(eV)	E_g(eV)
TiO2	-0.29	2.91	3.32
In2S3	-0.93	-1.23	1.58
PANi (polyaniline)	-1.67	-0.73	2.4

1. *Effect of seed layers on TiO2 nanorod growth on FTO for solar hydrogen generation. Hyun Kim, Bee Lyong Yang. International Journal of Hydrogen Energy 40(2015) 5807-5814.*

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-500**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Fabrication of ZnO-ZnS@polyaniline nanohybrid on FTO glass for enhanced Hydrogen generation

김현 양비룡*

금오공과대학교 신소재공학과

Heterojunction structures are attracting lots of attention for enhancing the electron injection across the interface. ZnO-ZnS@polyaniline one-dimensional nanohybrid films are synthesized on conducting glass substrates in a controlled way, using a simple three-step electrochemical deposition, chemical sulfurization of ZnO nanowire array as reactive template and spin-coating technique. The Electrochemical measurements were performed using a 1 kW xenon lamp (Newport) with its infrared wavelengths filtered out by water, and wavelengths below 420 nm removed by an optical filter, enabling measurements under visible light. The light irradiance, measured by a thermopile detector, was 100 mW/cm^2. A monochromator (74,000, Newport) was used to investigate the monochromatic responses (for IPCE, applied bias photon to current efficiency (ABPE), and band gap energy measurements) of samples. [1] The as-prepared ZnO-ZnS@polyaniline one-dimensional nanohybrids are found to exhibit significantly an enhancement in the incident photon-to-electron conversion efficiency as compared to ZnO nanowire arrays. The observed enhancement in photoelectrochemical activity is attributed to the photosensitization effect of visible light responsive PANI. The special electron structure in the heterojunction helped to reduce the energy barrier height at the interface and enhanced the separation of photo-generated carriers. Thus, the photoelectrochemical performance and the dispersing stability of the composite photocatalysts in water were highly improved. Hence, our proposed structure is a promising candidate as a photoanode for solar energy-to-hydrogen conversion devices.

Figure 1: show potential energy level ZnO-ZnS@polyaniline one-dimensional nanohybrid, relative to the redox potential for water splitting

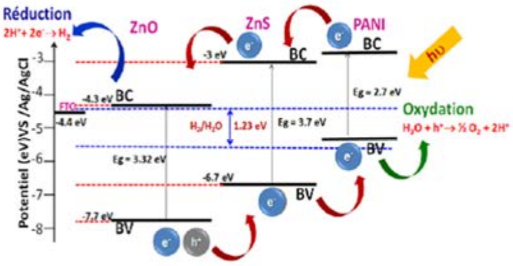


Table 1. Energy of band edge and gap

Materials	E_C(eV)	E_V(eV)	E_g(eV)
ZnO	-4.3	-7.7	3.32
ZnS	-3	-6.7	3.7
PANi (polyaniline)	-2.77	-5.23	2.7

1. *Effect of seed layers on TiO2 nanorod growth on FTO for solar hydrogen generation. Hyun Kim, Bee Lyong Yang. International Journal of Hydrogen Energy 40(2015) 5807-5814.*

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **MAT.P-501**
발표분야: 재료화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Light-triggered Drug Release and Photothermal Therapy using Gold Nanorods

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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 can penetrate tissues 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: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC.P-502**

발표분야: 전기화학

발표종류: 포스터, 발표일시: 금 13:00~14:30

Metal-encapsulated organic lead halide perovskite photocathode for photoelectrolysis of water

Mai Thi Kim Cuc 오일환[1,*]

금오공과대학교 IT 융합공학과 [1]금오공과대학교 IT 융합공학과, 금오공과대학교 응용화학과

The using solar energy to produce hydrogen by means of water splitting process is one of the most interesting ways to achieve clean and renewable energy. The rapid improvement of perovskite solar cells (PSCs) has made them the biggest interest to be studied for application in many fields, including employing in water splitting. However, PSCs are highly susceptible to degradation by moisture and water.Herein a simple method that enables the stability of perovskite device for photoelectrocatalyst hydrogen evolution in water is reported. Field’s metal, a fusible InBiSn alloy, is used efficiently as a protection layer to block electrolyte from attacking underlying perovskite layer while simutaneously allowing the photogenerated electrons to reach a hydrogen evolution catalyst. The photoelectrodes show remarkable stability retaining more than 8 hours under continuous illumination.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-503**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Development of novel electrolytic salts for high voltage Electrical Double Layer Capacitors

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군산대학교 화학과

EDLC is a high-power, high-stability energy storage device that expresses capacitance via electric double layers.However, the energy density per volume is low. An effective way to improve energy density is to improve the operating voltage. There is a limit to the oxidation stability of solvents, cations, and anions, which are the constituents of the electrolytic solution. Therefore, there is a request to develop novel electrolytic salts that can be used at higher voltages than existing electrolytic salts. In this research, we synthesized novel electrolytic salts with high purity, the properties new salts were studied with electrochemical evaluation methods. The new electrolytic salts were dissolved in the acetonitrile solvent. EDLCs using kinds of electrolytes were evaluated with maximum proposed operating voltage of 3.1V or higher in order to investigate about the oxidation decomposition of these kinds of novel electrolytes at high certain voltages. The cations salts were synthesized and the anions of cations salts were ion-exchanged with the commercial electrolytic salts which are used popularly in lithium-ion batteries. After synthesizing novel electrolytic salts, 1 H-NMR and 13 C-NMR measurements were used to confirm the synthesis. The novel electrolyte salts were evaluated with EDLC to investigate about the Coulumbic efficiency and discharge capacitance were measured according to the voltage step mode, and the performance were compared with the existing electrolyte salts up to now.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-504**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Influence of Additives on Organic Solvent-based Electrolyte for Electrochemical Double-Layer Capacitors

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군산대학교 화학과

Electrochemical Double-Layer Capacitors (EDLCs), also called capacitors, it has a wide range of application such as electrical energy storage systems, hybrid electric vehicles (HEVs), portable devices and for storage of energy generated by solar cell. Commercial EDLCs have activated carbon (AC) as the generally used electrode material because of its great adsorptivity and high surface area compared to the other materials. EDLCs has higher power density but lower energy density than those of rechargeable batteries. Because the operative voltage of capacitors is related to the specific energy of EDLCs: (E=1/2 C·V^2), it is important to increase the voltage of the capacitors for improved energy storage. But, there is one issue, at high voltages, the component of electrolyte (organic solvents) tend to decompose, leaving a highly resistive surface film on the electrodes. In this paper, we will focus on research about the influence of Additives on Organic Solvent-based Electrolyte to electrodes, that is the formation of Solid Electrolyte Interphase (SEI) on the surface of electrodes to mitigate the electrolyte decomposition and reactions of electrolyte to the surface of electrode as well as suppress the increase of the charge transfer resistance. Therefore, it will improve the electrochemical performance of EDLCs during cycling. Spiro-1,1’-bipyrolidinum tetrafluoroborate (SBP-BF4), a spiro-type quaternary ammonium salt, has a low viscosity and a high solubility in various solvents. Furthurmore, it shows excellent electrochemical stability and a high conductivity. In the present study, it was expected that additives would increase the ionic conductivity and the mobility in the electrolyte that would allow faster charge/discharge and better performance for EDLCs.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-505**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Effect of Roughness of Flat Nanoporous Pt Layers on Electrocatalytic Oxygen Evolution Reaction

임태정 김종원*

충북대학교 화학과

태양열, 풍력, 지력 등의 천연에너지에서 전기 에너지를 공급받아 물을 분해하여, 전기를 화학적 에너지로 저장하는 물 분해 전지는 최근 큰 각광을 받고 있다. 하지만 전지의 핵심 반응인 산소 발생 반응(OER)은 높은 과전압을 가지며, 이는 실용화에 가장 큰 걸림돌로써 작용한다. 따라서 OER 의 과전압을 낮추는 연구가 최근 활발히 진행되고 있다. 백금은 귀금속(noble metal)에 속한 금속이며, 귀금속은 일반적으로 OER 에 대해 높은 활성을 보인다. 특히 백금은 높은 전압을 필요로 하는 OER 동안 거의 녹아 나오지 않아, 높은 내구성을 가진다는 장점을 가지고 있다. 본 연구에서는 전기화학적 석출을 통해 평평한 표면의 나노 다공성 백금 층을 형성하여 표면에서의 OER 활성을 관찰하였다. 관찰한 나노 다공성 구조들은 형성 전하량을 증가시킬수록, 표면에 큰 구조적 변화 없이 층의 높이와 표면적이 증가하였다. 또한 구조의 표면적 증가와 OER 활성 증가가 비례하는 것을 관찰하였다. 특히 가장 높게 층을 형성하였을 때, 10 mA cm^{-2} 에서 1.566 V (vs. RHE)의 낮은 OER 과전압을 보여주었다. 또한 tafel slope 가 bulk Pt 대비 20 mV/dec. 증가하여, 나노 다공이 OER 에 필요한 전자전달을 빠르게 하여 과전압을 낮추는 것을 관찰하였다. 구조의 나노 다공이 OER 활성에 주는 영향을 관찰하기 위해 나노 다공을 50% 가량 유착시킨 구조들과, 유사한 표면적을 가지는 다른 백금 구조들에서 OER 활성을 관찰하였다. 두 실험의 결과로써, 구조의 높은 OER 활성은 나노 다공에서 기인함을 확인하였다. 본 연구의 결과는 OER 에 대해 높은 활성을 가지는 기판을 손쉽게 형성하는 방법을 제시하였고 나노 다공은 표면적을 증가시킬 뿐만 아니라, OER 활성을 증가시킬 수 있다는 것을 실험적으로 관찰하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-506**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

The Effect of Halide on the Pt Nanoparticles and Their Electrocatalytic Performance for Oxygen Reduction Reaction

박현욱 박아현 정종운 권영욱*

성균관대학교 화학과

In the present work, we have synthesized Pt/C_KX (X = I, Br and Cl) samples in which 5 ~10 nm sized Pt nanoparticles (NPs) on a carbon support by an one-pot ultrasound-assisted polyol synthesis (UPS) method 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, Br and Cl) samples, Pt(acac)2, KX (X = I, Br and Cl) and carbon support were dispersed in 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, electrochemical surface areas (ECSAs) and ORR activity of Pt/C_KI sample are inferior to that of commercial Pt/C in acid media. We assumed that it could be caused by poisoning of iodide from KI resulting in block the surface of Pt NPs. Interestingly, ORR activity of Pt/C_KBr sample is superior to that of commercial Pt/C in acid media. It means that bromide can lead to the enhanced electrocatalytic activity in ORR. Therefore, we found that the effect of halide on the Pt NPs are different in each type of halide. In conclusion, we demonstrated that the halide effects on Pt NPs can increase or decrease the electrocatalytic performance and durability.

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장소: 일산 KINTEX
발표코드: **ELEC.P-507**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Switchable photovoltaic effect in lateral and vertical structure organometal trihalide perovskite solar cells

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Recently, the use of organometal trihalide perovskite (OTP) as light absorber in solar cells has increased rapidly because of its low-cost, easy fabrication and high power conversion efficiency (PCE). Here, we show that, in both OTP vertical and lateral photovoltaic devices, the direction of the diode polarity and the photocurrents can be reversed repeatedly by applying a small electric field of < 1V μm-1. The ionic electromigration in perovskite layers induces the formation of reversible p-i-n structure, which has been identified as the origin of the switchable photovoltaic effect. The best device parameters in the poled single-layer vertical devices are comparable to those of optimized multi-layer devices with both electron- and hole-transporting layers. The lateral devices are particularly interesting because the device cost can be reduced significantly by eliminating the need for transparent electrodes. Moreover, a higher voltage can be obtained by connecting lateral structure devices in series, which meets the needs of many applications, such as house-hold devices (110 V), battery chargers (12 V), etc. This study provides a novel method for designing perovskite solar cell and manipulating the electric properties of perovskite film.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-508**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Ultrasound-Assisted Syntheses of Extremely Small and Amorphous NiFe-based Nanoparticles as Superior Electrocatalysts for Oxygen Evolution Reaction

박아현 박현욱 정종운 권영욱*

성균관대학교 화학과

In this study, we present the one-pot syntheses of NiFe-based nanomaterials and their electrochemical performance for oxygen evolution reaction (OER) in alkaline media. By using a simple sonochemical route, we achieved the preparation of amorphous and composition tunable NiFe-based nanomaterials which are received lots of attentions as desirable and novel electrocatalyst with low overpotential for OER. Through the structural characterization, we found that these materials have extremely small particle size and homogeneous elemental compositions. Electrochemical analysis also showed that the OER activity of samples exhibit the volcano-type trend according to adjusting of Fe content. Among them, $Ni_{70}Fe_{30}$ sample showed overpotential of 292 mV at 10 mA cm^{-2}_{geo} and Tafel slop of 30.4 mV dec^{-1}, which outperform that of IrO_x/C (326 mV, 41.7 mV dec^{-1}). Chronopotentiometry at 10 mA cm^{-2}_{geo} for 2 h of samples for durability test reveals that $Ni_{70}Fe_{30}$ sample maintains the steady-state potential compared with that of IrO_x/C, meaning an excellent durability of our samples. Based on our results, we demonstrated that sonochemical syntheses could be novel approach to prepare superior and durable OER electrocatalyst with for water electrolysis and metal-air battery.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-509**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Effect of structure and Ir modification at porous Pt structures on electrocatalytic oxygen evolution reaction activities

성문창 김종원*

충북대학교 화학과

산소 발생 반응은 외부의 다른 형태의 에너지(전기, 빛 등)를 화학 에너지 형태로 저장하는 전기 화학 장치에서 발생하는 반응이다. 이 전기 화학 장치는 물 분해 반응을 이용하는데, anode 에서는 산소 발생이 일어나고 cathode 에서는 수소의 발생이 일어난다. 특히 산소 발생의 경우 반응이 매우 느리게 일어나는데, 따라서 높은 과전압이 요구 되는 문제가 있다. 따라서 여러 연구들에선 이 과전압을 낮추기 위한 방향으로 많은 연구들이 진행되고 있다. 본 연구에서는 백금 구조의 모양에 따른 산소 발생 반응 활성의 영향을 관찰 하였다. 백금 구조는 전기화학적 석출 방법을 이용하여 구조를 만들었다. 전기화학적 석출 방법을 통해 걸어주는 전압과 조건을 달리하여 구조를 다르게 조절할 수 있다. 특히 본 연구에서 구조의 변화를 주기 위해 매끈한 표면의 Pt ball 과 거친 표면의 Pt ball 을 만들었으며, 각각 SEM 을 이용하여 구조를 확인 하였다. 나아가 Ir 이 자발적으로 백금에 치환되는 것이 관찰되었고 이를 이용하여 산소 발생 반응의 활성에 어떤 영향을 미치는지 알아보았다. Ir 의 치환 여부는 EDX 와 XPS 를 통하여 Ir 의 석출을 알 수 있었다. 또한 SEM 을 통해 구조적인 변화는 없다는 사실도 확인 하였다. 이런 전극들을 활용하여 산소 발생 반응에 대한 활성의 변화를 비교하였고, 그 결과 Pt ball 의 porosity 가 증가 할수록 산소 발생 반응에 대한 활성이 좋아졌으며, Ir 을 치환 시켰을 경우에는 훨씬 산소 발생 반응에 대한 활성이 증가하였다. Pt ball 표면의 거칠기 또한 산소 발생 반응에 영향을 미쳤으며, 이는 Pt 의 구조가 산소 발생 반응에 영향을 미치는 사실을 알 수 있었다. 또한 활성이 매우 증가한 Ir 이 치환된 Pt 구조의 경우는 구조에 큰 영향이 없이 일어났으며, Ir 의 자발적인 치환은 Pt 구조와는 상관없는 현상으로 보인다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-510**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Simple Syntheses of Silicon/Titania Nanocomposites on Copper Foils as Lithium-ion Battery Anodes

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Combining advantages of high specific capacity and a very small volume expansion ratio, Si/TiO_2 nanocomposites are considered as a promising candidate material for lithium-ion battery anodes. In our recent work, highly porous wire-like TiO_2 nanostructures with silicon nano-coating as lithium-ion battery anodes have been synthesized directly onto copper foils by a simple two-step process. [1] Firstly, interconnected TiO_2 nanowires are synthesized onto the surface of copper foil by an alkali-hydrothermal route. [2-5] Subsequently, Si is deposited onto the surface of the nanowires, forming a silicon/TiO_2 nanocomposite (denoted as Si/TNW composite). The morphological and structural characterizations were investigated by SEM, XRD, EDS, and RAMAN, revealing that the TiO_2 wires typically have lengths from 200 nm to 400 nm and widths from 20 nm to 50 nm and the Si has a flattish surface with thicknesses of 100, 200 and 300 nm deposited on TiO_2 nanowires. These characteristic results indicated that the resulting Si/TNA composites have potential to apply for lithium-ion battery anodes.References:1. T.W. Pat. No. I491577 Chen, J. Z.; Yen, Y. C.; Chen, P. H.; Lin, K. J. 2015-20362. 2. Chen, J. Z.; Ko, W. Y.; Yen, Y. C.; Chen, P. H.; Lin, K. J.* ACS Nano. 2012, 6, 6633-6639.3. Yen, Y. C.; Chen, J. Z.; Lu, Y. J.; Gwo, S.; Lin, K. J.* Nanotechnology. 2014, 25, 235602-235609.4. Chen, J. Z.; Yan, Y. C.; Ko, W. Y.; Chen, C. Y.; Lin, K. J.* Adv. Mater. 2011, 23, 3970-3973.5. Yen, Y. C.; Ko, W. Y.; Chen, J. Z.; Lin, K. J.* Electrochim. Acta 2013, 105, 142-148.

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발표종류: 포스터, 발표일시: 금 13:00~14:30

Stable Performance of Aluminum Metal Battery by Incorporating Lithium Ion Chemistry

유동주 최장욱[1,*]

KAIST EEWS 대학원 [1]KAIST EEWS

Based on the recent discovery of the ionic liquid involving $AlCl_4^-$-$Al_2Cl_7^-$ redox couple as an electrolyte, aluminum (Al) rechargeable batteries have received revamped interest. However, the corrosive nature of the chloride ion and $Al_2Cl_7^-$ makes it challenging to find suitable current collectors and cathode materials. Here, we screen various metals and carbon materials as current collectors, and indeed find that none of the metals commonly used for battery current collectors is stable against corrosion from the electrolyte. Only pyrolytic graphite is stable, but exhibits undesired $AlCl_4^-$intercalation at 1.7 V vs. Al/Al^{3+}. The addition of lithium chloride (LiCl) salt to the electrolyte not only eliminates the $AlCl_4^-$ intercalation via the Li─$AlCl_4^-$coordination but also extends the stable voltage window to 2.3 V vs. Al/Al^{3+}. Moreover, the incorporation of Li ions allows us to engage the established $LiFePO_4$ olivine cathode in Li-ion batteries. This Al-Li hybrid cell exhibits an operation voltage of 1.3 V with robust cyclability (83.4 % retention after 400 cycles) and minimal self-discharge. This series of results suggest that proper employment of Li ion chemistry can improve electrochemical performance and safety of Al rechargeable batteries.

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Spontaneous synthesis of silver nanoparticles using carbon dots and their electrocatalytic application

임호섭 심준호*

대구대학교 화학과

Carbon dots (CDs), mainly consisting of a graphite structure or amorphous carbon core and carbonaceous surfaces with rich oxygen-containing groups, have attracted tremendous interest because of their unique properties, including high surface area, superior electro-optical properties, high water solubility, and high chemical stability. In this presentation, a stable silver nanoparticles/CDs composite was prepared by using CDs as reducing and stabilizing agent. To the best of our knowledge, the use of CDs as reducing and stabilizing agents has rarely been reported in conjunction with their use in the fabrication of silver nanoparticles. The electrocatalytic activity of the silver nanoparticles/CDs for oxygen reduction and oxygen evolution reaction in alkaline media was investigated by rotating disk electrode, and cyclic voltammetry. Indeed, the resultant silver nanoparticles/CDs composite exhibited good catalytic activity for the reduction of oxygen, compared with the silver nanoparticles synthesized by citrate reduction. The compositional/structural features are characterized by high-resolution transmission electron microscopy, Fourier transform infrared and UV-Vis spectroscopy, and X-ray photoelectron spectroscopy. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2014R1A1A2054826 and 2016R1D1A1B03930895).

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Cobalt-iridium bifunctional electrocatalyst for oxygen reduction and oxygen evolution reactions

노승욱 박성철 심준호*

대구대학교 화학과

This presentation reports the facile synthesis and characterization of highly porous hollow Co-Ir nanostructures. The formation of porous Co-Ir nanostructure is through galvanic replacement with hollow cobalt mesospheres as the templates in metal ion precursor solutions. This approach does not require the further removal of templates and greatly simplifies the synthetic procedures. The porous Co-Ir nanostructures can be used as supportless electrocatalysts that exhibit enhanced catalytic activities in the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). The compositional/structural features are characterized by scanning electron microscopy equipped with an energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. The electrocatalytic activity of the Co-Ir for ORR and OER in alkaline media was investigated by rotating disk electrode, rotating-ring disk electrode, and cyclic voltammetry. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2014R1A1A2054826 and 2016R1D1A1B03930895).

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Spontaneous Phase Transition of Hexagonal Wurtzite CoO: Application to Electrochemical and Photoelectrochemical Water Splitting

장규연 남기민[1,*]

목포대학교 화학화 [1]목포대학교 화학과

Herein we report the spontaneous phase transition of h-CoO to Co(OH)2 in deionized water, and their application to the water splitting reactions. The addition of water drives the phase transition of the h-CoO to Co(OH)2 nanocrystals. Interestingly, the non-native h-CoO only progressed in the phase transition reaction to Co(OH)2 in the presence of water. The phase transition is unfavorable in the case of c-CoO nanocrystals. Moreover, performing the phase transition of h-CoO on various substrates results in efficient chemical bonding between the Co(OH)2 and substrate without additional processes. The proficient interaction of Co(OH)2 on the substrate is suitable for application to the catalytic water oxidation reaction.

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Temperature Dependent Crystal Structure of MoO3 for Sodium-Ion Batteries

정은지 손용근*

성균관대학교 화학과

Secondary battery systems are considered as an essential energy storage systems (ESSs). Among them, Li-ion battery (LIB) is recognized as the best one right now. Because they are already proved their capability of ESS for small portable devices as well as some of grid systems. However, Li which is the main material of LIB has limited supply because the Earth's crust runs out thus the cost of lithium is increasing. Sodium, the second lightest alkali metal next to lithium, attracts researcher's interest as an alternative choice because sodium is one of the most abundant materials and easily found on the earth. For large-scale energy storage systems, many great studies have made progress in exploring capable Na cathode. However, only a few anode systems have been investigated. Therefore, research work about favorable anode material is important in development of sodium-ion batteries (SIBs). As an anode material for SIBs, molybdenum-based materials were used because they have many advantages such as low cost, abundant resources and non-toxicity. In this work, nanobelt and hexagonal prism structured MoO3 were successfully synthesized by hydrothermal method for SIB use. The structures of MoO3 were dominantly influenced by the synthetic hydrothermal temperature. This temperature also affects the crystallinity of MoO3. Nanobelt and hexagonal prism structures were characterized by Scanning electron microscope (SEM), X-ray Diffraction (XRD), Energy dispersive X-ray spectroscopy (EDS). Electrochemical properties were measured by Cyclic Voltammetry (CV).

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Electrocatalytic Activities of Highly Dispersive Gold Nanoparticles on Carbon Black

김여민 조아라 이영미* 이종목*

이화여자대학교 화학나노과학과

We investigated electrocatalytic activities toward oxygen reduction reaction (ORR) and CO_2 reduction with highly dispersive gold nanoparticles on carbon black (HD-AuNPs/C). The catalysts were synthesized through a facile chemical reduction method in aqueous solution. The dispersity and size of Au NPs on carbon black were controlled by varying the concentration of reducing agent, where the mean diameters of Au NPs on carbon black were changed from 1.4 to 6.0 nm. HD-Au NPs/C with mean diameter of 1.4 nm Au NPs exhibited the best catalytic performance for ORR in the rotating disk electrode experiments having the electron transferred number of 3.61 and the most positive half-wave potential which was comparable with Pt/C. Meanwhile, the cyclic voltammetry (CV) experiments showed CO_2 reduction preceded hydrogen evolution reaction in HD-Au NPs/C as the potential moved to the negative direction. Generation of CO, the reduction product of reduction of CO_2, was also monitored in real time during CV using substrate generation/tip collection (SG/TC) mode of SECM, where the Pt/Sn CO microsensor were used as a tip electrode.

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Cobalt and silver electrodeposition as an efficient oxygen reduction reaction electrocatalyst

문신영 이영미[1,*] 조윤빈[1]

이화여자대학교 화학.나노과학과 [1]이화여자대학교 화학나노과학과

Oxygen reduction reaction (ORR) is one of the sluggish reactions that occur in fuel cells. Although platinum (Pt) and its alloy materials are the best catalysts for ORR, its high cost and limited amounts make commercial uses of Pt difficult. Among the non-Pt-based electrocatalysts for ORR, silver (Ag) is a well-known alternative to Pt with low price and the fine catalytic activity of reducing oxygen through the direct four-electron transfer reaction. To decrease the overpotential and enhance the activity of Ag in alkaline media, the weak binding of the oxygen atom to Ag surface in the first step of ORR (O-O bond cleavage) can be improved by mixing Ag with cobalt (Co). Cobalt helps the O-O bond breakage and then Ag reduces the resulting adsorbed atomic oxygen. In this work, Ag and Co are electrodeposited on glassy carbon rotating disk electrode (GC-RDE) simultaneously and their electrocatalytic activity for ORR is studied by varying the atomic ratio of Ag and Co. 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 both 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).

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Fabrication of a Dual Microsensor for Simultaneous Measurements of Carbon Monoxide and Potassium Ion

우주원 이영미*

이화여자대학교 화학나노과학과

Carbon monoxide (CO) and potassium ion (K^+) are significantly related to vasodilation and neurotransmission in physiological systems. 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 aroused by K^+ channel existing in neuron cells. In this presentation, the development of a dual amperometric microsensor for simultaneous measurements of CO and K^+ is demonstrated. A working electrode of the sensor is a dual disk electrode having platinum (Pt) and silver (Ag) microdisks (diameter of both disks, 76 μm). Both Pt and Ag microdisks are electrochemically etched to form dented micropores. Pt micropore is filled with porous bimetallic layers electrodeposited sequentially. Then, the electrode surface is modified with electropolymerized polymer and CO selective membrane for the selectivity to CO over general biological interfering species. Ag micropore is chloridated with $FeClH_3$ to form AgCl, followed by silanization with trimethylchlorosilane (TMCS), and then covered with K^+ selective membrane. The sensitivity and selectivity of the dual sensor are experimentally verified for possible 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).

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Controlling platinum microstructures on electrodes for simple and selective amperometric sensing of nitric oxide

김소희 이영미*

이화여자대학교 화학나노과학과

Nitric oxide (NO) is known as an important gaseous signaling molecule in biological systems, playing roles as vasodilation, immune response, and neurotransmission. Therefore, real-time simultaneous detections of NO *in vitro/vivo* are valuable in medical and biological sciences. Electrochemical sensors have advantages of *in situ* and/or real time NO measurements. However, a variety of biological interferents including anionic ascorbic acid, neutral acetaminophen and cationic dopamine can be oxidized at potentials required to detect NO based on the oxidation. Several ways have been tried to reduce the interruption from these interferents with selective membranes such as chloroprene, PTFE (polytetrafluoroethylene), fluorinated xerogel and Nafion. In this research, we studied a simple fabrication method of a selective NO sensor by controlling surface microstructures of platinum (Pt) electrodes. Different morphologies of Pt nanoparticles were electrodeposited on a gold (Au) disk electrodes (diameter, 2 mm) depending on the concentrations of Pt precursors. The morphologies and compositions of the deposited Pt nanoparticles were characterized by field-emission scanning electron microscopy (FE-SEM). Also, water contact angles with drops of deionized water on the electrodes were measured to investigate the hydrophobicity of the electrode surfaces (IMAGE J). Amperometric responses of the electrodes to NO and interferents were obtained at +0.75 V versus Ag/AgCl. The more hydrophobic structure exhibited the higher selectivity 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).

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Dual graphite cells for potassium-ion batteries

박춘국 표명호*

순천대학교 인쇄전자공학과

Graphite is known to be reliable anode materials in Li-ion batteries (LIBs). Graphite also has been studied as a cathode material in LIBs. As the requirement of development of next-generation batteries, however, graphite is also seeking for its use in a new system. The work using graphite in potassium ion batteries (KIBs) was triggered by the finding that potassium ions could be intercalated into graphite, in contrast to sodium ions. Graphite can also be used as a cathode in KIBs. When used as a cathode, the cations in electrolytes are intercalated into the anode, and the graphite cathode stores the anions of electrolytes. The process is reversed during the discharge step. However, the graphite is oxidized at high voltages (>5.0 V vs. K/K^+), which requires the careful selection of electrolytes. The electrolyte not only needs to be electrochemically stable at high potentials, but also to form stable SEI on an anode surface. In this study, we optimized electrolyte systems operable for K^+-based graphite dual-ion cells. We also tried to maintain the electroactivity of graphite anode which was usually blocked due to SEI formation. The composition of SEI layer on the graphite anode surface was investigated using XPS analysis. Based on these results, we are trying to construct a symmetrical full cell using graphite as the active materials.

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Comparison of electrochemical property of Mo_6S_8 in various electrolytes

<u>IKHE AMOL BHAIRUBA</u> 표명호*

순천대학교 인쇄전자공학과

Magnesium (Mg) ion batteries are one of the promising candidate systems to possibly surpass the volumetric density of LIBs, suppressing lithium dendritic growth, because Mg possesses two valence electrons and has a low standard reduction potential (-2.37 V vs. SHE). However, there are two major issues in developing the magnesium rechargeable batteries, which are: (i) slow diffusion of Mg^{2+} ions in active materials; (ii) relatively narrow potential windows of Mg^{2+}-based electrolytes. The first successful magnesium deposition/dissolution in Mg^{2+} electrolytes was reported by Aurbach group, using Mg organohaloaluminate salts. Inspired by this seminal work, researchers tried to increase the potential window (up to 2.3 V vs. Mg in APC-type) and to replace the toxic Grignard-based electrolytes. Various common electrolytes such as $Mg(TFSI)_2$, $Mg(ClO_4)_2$, Mg(TFS), and $MgCl_2$ and their combinations were reported to show higher anodic limits and reversible Mg^{2+} insertion/deinsertion in/out of Mo_6S_8. Herein, we also reports several combinations of common magnesium salt in ether type solvents to achieve high anodic limit, reversible Mg plating/ stripping, and reversible Mg^{2+} insertion/deinsertion for Mo_6S_8. The systems we evaluated as electrolytes for MIBs are: $Mg(TFSI)_2$:$MgCl_2$/THF (glyme families), $Mg(TFS)_2$:$MgCl_2$/ THF (glyme families), $Mg(TFSI)_2$:$AlCl_3$/ THF (glyme families), and more. Electrochemical stability of these electrolytes and electroactivity of Mo_6S_8 will be presented.

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One-Pot Synthesis of the Li_3VO_4 with Nitrogen-Doped Carbon Coating Layers as an Anode Material for Lithium-Ion Batteries

박한솔 박미지 김종식*

동아대학교 화학과

Lithium-ion batteries (LIBs) have been utilized as effective power supplies for a wide range of application such as laptops, mobile phones, and cameras owing to low cost, high capacity, and long life cycles. Nevertheless, because graphite has a low theoretical capacity (372 mAh g^{-1}), it is necessary to explore an 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. Lithium vanadate (Li_3VO_4) has been recently investigated as a potential anode material for lithium-ion batteries (LIBs) because it has advantages of high theoretical capacity of 394 mAh g^{-1}, small volume changes, and fast diffusion of lithium ions during charge/discharge processes. However, pristine Li_3VO_4 (LVO) has a low initial Coulombic efficiency and poor electrochemical performance (especially poor rate capacity) because of its low electrical conductivity. In this work, the nitrogen-doped carbon coated Li_3VO_4 (NC-LVO) was successfully fabricated via facile hydrothermal and subsequent heat treatment methods using dopamine (2-(3, 4-dihydroxyphenyl)ethylamine) which includes nitrogen and carbon functional groups. Compared with the pristine LVO, the NC-LVO sample showed enhanced the electrochemical performances with the reversible capacity of about 426 mAh g^{-1} with a capacity fading rate of about 0.024% per cycle during the 2-100 cycles at 0.5 C (1 C = 394 mA g^{-1}) in the voltage ranges of 0.01-3.0 V. Furthermore, the NC-LVO also exhibited the improved initial Coulombic efficiency with about 70% and rate capabilities at various current densities (0.1-20 C).

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Self-Assembled Rose-Shaped ZnO Microstructures as an Anode Material for Lithium-Ion Batteries

김한아 김남영 김종식*

동아대학교 화학과

Zinc oxide (ZnO) has attracted significant attentions as an alternative anode material for lithium-ion batteries (LIBs) because of its high theoretical capacity (987 mAh g^{-1}), non-toxic, abundant, and environmental friendliness. Especially, its theoretical capacity is about three times higher than that of the commercialized graphite anode (about 372 mAh g^{-1}) through the alloy and conversion reactions of ZnO with lithium ions. However, severe capacity fading and poor reaction kinetics are caused by low electrical conductivity, slow diffusion of lithium-ion, and large volume changes during charge/discharge processes of ZnO. To overcome these drawback, many studies have been reported about utilizing coatings or mixing with conductive materials to enhance the conductivity and promote the electrochemical reactions. In this work, N-doped carbon-coated ZnO microstructures (ZnO/NC) were synthesized through a facile hydrothermal reaction using urea and citric acid as nitrogen and carbon sources, respectively. The ZnO/NC sample has self-assembled rose-shaped microstructures, which are composed of primary nanoparticles. It exhibited a higher discharge capacity of about 1047 mAh g^{-1} after 100 cycles at a rate of 0.1 C in the voltage range of 0.01-3.0 V, compared to those of bare ZnO and carbon-coated ZnO (ZnO/C) samples (about 42 mAh g^{-1} after 50 cycles and 341 mAh g^{-1}, respectively).

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리튬-이온 배터리 양극재료 NCM의 충·방전에 따른 상변태 및 격자 변형량의 상관관계

김준동 박정희[1,*] 안재평[2,*]

고려대학교 신소재화학과 [1]고려대학교 소재화학과 [2]한국과학기술연구원(KIST) 산업화지원센터

NCM 으로 불리는 Li(NiCoMn)O_2 은 차기 리튬 이온 배터리 분야에서 가장 중요한 양극 물질이다. 기존의 리튬 이온 배터리 물질에서 쓰이고 있는 $LiCoO_2$ 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 삽입·탈리에 대해 지금까지 직접적으로 규명한 사례는 극히 제한적이다.본 연구에서는 투과전자현미경에서 나노회절패턴과 전자 빔의 세차회절 방법을 동시에 사용하여 상변화와 격자변형을 측정함으로써 NCM 의 열화 원리를 연구하였다. 상변형에 대해 ASTAR, 격자변형에 대해 TOPSPIN 을 사용하여 측정 및 해석하였다. 이 방법은 2 nm 의 매우 작은 영역만을 회절시켜 양극입자의 어떤 부위라도 국부적인 나노 회절패턴을 얻고 해석할 수 있다. 또한 2 nm 이하의 전자빔을 스캔하여 특정 면적에 대해 10~20 만장 정도의 나노 회절패턴을 매트릭스 형태로 측정하여 분석하기 때문에 기존의 HRTEM 이미지와 SAD 패턴의 단점이었던 해석의 모호성을 제거할 수 있는 장점을 갖고 있다. 이러한 결과는 배터리 용량감소 분야에 기여할 것으로 생각된다.

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장소: 일산 KINTEX
발표코드: **ELEC.P-525**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Determination of superoxide dismutase (SOD) with lucigenin electrogenerated chemiluminescnece (ECL) at mesoporous platinum electrode

남성주 이원용*

연세대학교 화학과

A simple method for the detection of SOD has been developed using the electrogenerated chemiluminescence (ECL) of lucigenin on a mesoporous platinum electrode. A mesoporous platinum electrode provides significant enhancement of the electrochemical signals for kinetic-controlled reactions since they are affected by the nanoscopic surface area of the electrode. For a diffusion-controlled reaction, however, the electrochemical signal is identical to that of a bare platinum electrode since reactants are depleted inside the mesopores. Such characteristics of a mesoporous platinum electrode provide highly enhanced signal for the anodic ECL of lucigenin in neutral solution system without the use of additional modifications to the electrode or further addition of other materials for signal enhancement. Superoxide dismutase (SOD) is an enzyme that plays an important role in nearly all living cells as it provides defense against oxidative damage from superoxide free radicals. Since a number of diseases, such as breast cancer, pancreatic adenocarcinoma, and papilloma, are known to be associated with the overexpression of SOD, quantitative analysis of SOD is required for the diagnosis of such diseases. Based on the capability of SOD to inhibit the anodic ECL of lucigenin by its inherent ability to catalyze the reduction of superoxide anions, a simple and sensitive ECL biosensor for the detection of SOD has been developed.

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Simple preparation and characterization of sponge-like graphene oxide/carbon nanotubes composites for supercapacitors

손영래 박수진*

인하대학교 화학과

Sponge-like graphene oxide/carbon nanotubes (S-GO/CNT) composites were prepared by integrating GO nanosheets and CNT via sonication and lyophilization. The as-prepared S-GO/CNT composites possess highly holey structure, leading to providing highly effective electrolyte pathway. Reduced S-GO/CNT (rS-GO/CNT) which can be used as electrode in supercapacitor can be prepared by annealing the S-GO/CNT composites without distinct deformation. The characterization of S-GO/CNT and rS-GO/CNT composites was investigated by X-ray diffractometer, transmission electron microscope and scanning electron microscope. The electrochemical measurements of rS-GO/CNT composites were performed by cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy. The rS-GO/CNT electrode possesses excellent rate capability and cycling stability owing to its high electrical conductivity and superior structural stability.

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Electrochemical Stability of Graphene Coated Current Collectors in Grignard Reagent-Based Electrolytes for Magnesium Ion Battery

S.J. Richard Prabakar 표명호*

순천대학교 인쇄전자공학과

The electrochemical stabilities of several non-noble metal current collector electrodes in a magnesium ion battery (MIB) using tetrahydrofuran solution containing phenylmagnesium chloride and aluminum chloride (Grignard reagent type electrolyte) was investigated. The cyclic voltammetry and chronoamperometry studies revealed pitting type corrosion on non-noble metal electrodes at high potentials, wherein the chloride ions were responsible, which eventually lowered the corrosion resistance. In this investigation, we explore the possibilities of graphene and functionalized graphene as protective coatings on the non-noble metal current collector electrodes. From cyclic voltammetry and chronoamperometry studies, the graphene (or functionalized graphene) coated non-noble metal electrodes showed considerable improvement in corrosion resistance, predominantly with a notable suppression of electrolyte oxidation at high potentials, without the deposition/stripping of Mg being affected. Studies showed a variance in the corrosion resistance which was dependent on the functional groups on graphene, coating effectiveness and thickness. We believe graphene coating to behave as a barrier to chloride ion permeation and prevent the corrosion of the underlying metal for longer periods. Additionally, graphene (or functionalized graphene) can diminish the microcracks and micropores of the metal surface to decrease the corrosive area. The results show that the graphene/functionalized graphene coated non-noble metal electrodes can be suitable replacements for the expensive Pt electrode in a corrosive Grignard reagent type electrolyte for MIB.

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The electrochemical catalytic reaction of PAA-PVI-[Os(4'4-disubtituted 2'2-bipyridines)2Cl]+/2+with glucose dehydrogenase

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단국대학교 화학과 [1]단국대학교 나노바이오의과학과

Screen printed carbon electrodes (SPCEs) with immobilized osmium-based hydrogel redox polymer, glucose dehydrogenase (GDH) and PEGDGE can be used to apply glucose electrochemical detecting. The osmium redox complexes were synthesized by the coordinating pyridine group having different functional group at 4-position with osmium compounds. The synthesized poly-osmium hydrogel complexes are described as poly(acryl amide)-poly(vinyl imidazole)-[Os(4,4'-disubstituted 2,2'-bipyridines)2Cl]+/2+ (PAA-[Os(4,4'-disubstituted 2,2'-bipyridines)2Cl]+/2+) polymers. The different concentrations of glucose were measured by cyclic voltammetry technique using enzyme-immobilized SPCEs. The resulting electrical currents displayed a good linear response with glucose concentrations with GDH. Therefore, this approach allowed the development of a simple, point of care in the medical field, disposable electrochemical biosensor.

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The electron transfer behavior of the glucose dehydrogenase based chitosan composites with multiwalled carbon nanotubes for determination of glucose

이보희 전원용[1] 최영봉 김혁한*

단국대학교 화학과 [1]단국대학교 나노바이오의과학과

The electron transfer of the glucose dehydrogenase (GDH) immobilized electrode which modified chitosan composites with mutiwalled carbon nanotubes (Chit-MWCNTs) was investigated through electrochemical method. MWCNTs were wrapped by Chit for dispersion in water soluble solution, and then Chi-MWCNTs adsorbed electrode was fabricated onto indium-tin oxide (ITO) electrode. And GDH enzyme for determination of glucose was loaded on the Chit-MWCNTs/ITO electrode. The GDH/Chit-MWCNTs/ITO electrode were dried without cross-linker. The electron transfer reaction of the GDH with electrode were observed using electrochemical techniques. Also, field emission scanning electron microscope (FE-SEM) was used for investigation of all electrode’s morphologies. The electrical signal of glucose was measured onto GDH/Chit-MWCNTs/ITO electrode by cyclic voltammetry (CV). The GDH/Chit-MWCNTs/ITO electrode shown that has a simple fabrication method, high sensitivity, low-cost, and fast electron transfer directly.

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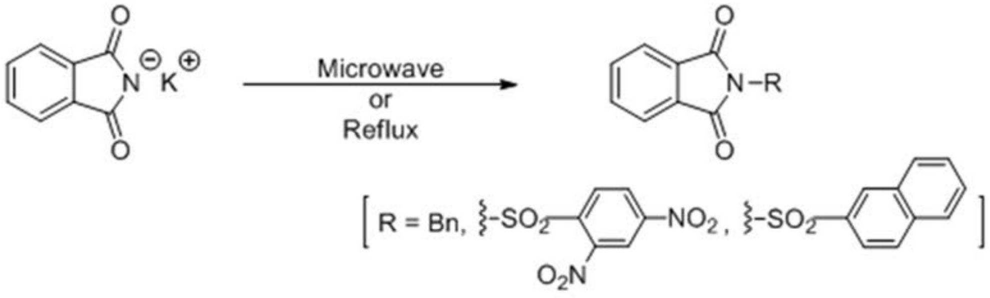
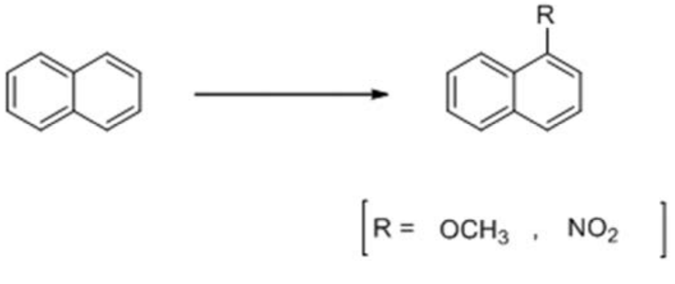
Preparation and Electrochemical Investigation of Phthalimide and Naphthalene Derivatives : Apply to Redox Flow Battery

이홍섭 안철진*

창원대학교 화학과

Recently phthalimide and naphthalene 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 naphthalene derivatives. To do this we prepared phthalimide and naphthalene derivatives and investigated CV results depending on their different functional group.





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Curvature-induced metal-support interaction of an islands-by-islands composite of platinum catalyst and carbon nano-onion for durable oxygen reduction

<u>양주찬</u>

UNIST 에너지공학과

Platinum nanoparticles supported by carbon (Pt/C) have been the most popular catalysts for cathodes of fuel cells. Du-rable operation of fuel cells based on Pt/C suffers from (1) loss of active Pt mass caused by carbon corrosion and (2) Pt particle agglomeration during operation. To address the issues of the conventional carbon supports, here we present carbon nano-onion (CNO), a new class of carbon allotrope, as a support for Pt catalysts. CNO had the spherical shape with 3 to 5 nm in diameter consisting of ~5 concentric graphitic layers. Superior durability of catalytic oxygen reduc-tion reaction (ORR) was guaranteed by Pt supported by CNO (Pt/CNO) due to: (1) the islands-by-islands configuration of the Pt/CNO composites (c.f. islands-on-a-particle configuration for Pt/C) to isolate each Pt nanoparticle from its neighbors by the same-size CNO particles and to suppress Ostwald ripening by highly tortuous void structure; (2) the curvature-induced strong interaction between CNO and Pt; and (3) the graphite-like concentric layers guaranteeing corrosion resistivity.

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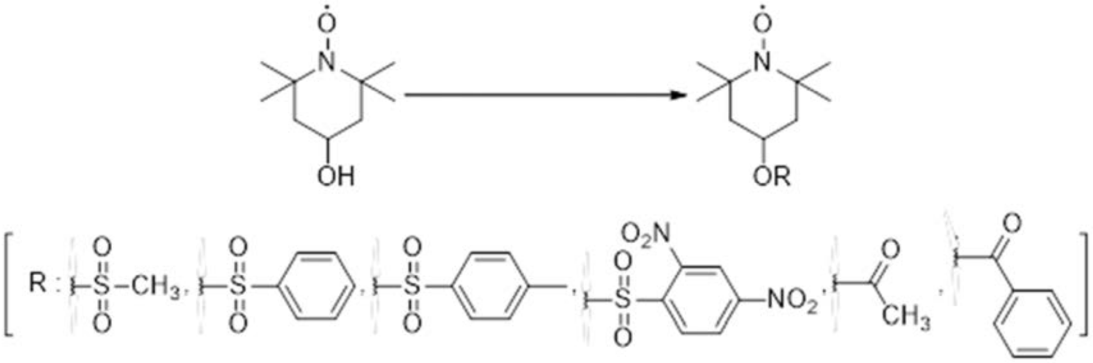
Preparation and Electrochemical Investigation of TEMPOL Derivatives: Apply to Redox Flow Battery

조현일 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.



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Nickel hydroxide supercapacitors based on 3D moss-like nickel current collectors

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We introduce a simple way to the realization of the theoretical specific capacitance and high rate capability of Ni(OH)2 supercapacitors, by utilizing a dendritic three-dimensional-nickel network current collector. A simple electrodeposition method was chosen for rapid fabrication of the dendritic 3D-nickel/copper structure. The inside residual copper moiety was selectively removed to generate the hollow dendritic 3D-nickel network current collector. After nickel hydroxide was deposited, it exhibited the highest capacitance of 3,637 F g-1 at a current density of 1A g-1, and retained 97% of capacitance at a high current density of 100 A g-1 with great cycle stability of over 80% after 10,000 cycles. When tested in a two electrode system, the energy density of 22.4 Wh kg-1 at a power density of 696.9 W kg-1 was achieved. These results offer a potential for state-of-the-art energy storage systems.

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Cascading Alignment of Multilayered $SnO_2/WO_3/BiVO_4$ Inverse Opal Skeletons in Photoelectrochemical Water Splitting

윤건 강순형[1,*]

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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, 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.

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An amperometric lactate biosensor based on porous carbon polymer composite

HUSSAIN KHALIL 심윤보*

부산대학교 화학과

Lactic acid plays an important role in cancer microenvironment and recently it emerged as a cancer biomarker for early diagnosis and prognosis of cancer, therefore, a sensitive and selective sensor is needed. In this study, an amperometric lactate sensor was fabricated by immobilizing lactate dehydrogenase (LDH) and nicotinamide adenine dinucleotide (NAD+) onto a layer composed of porous carbon and 3-([2,2':5',2"-terthiophen]-3'-yl)-5-aminobenzoic acid (TTABA) composite. Morphology and performance were investigated using SEM, XPS, EIS, QCM and cyclic voltammetry. The calibration plot at optimized experimental conditions showed a linear range of 0.5nM to 4mM. The reliability of the proposed sensor was evaluated in different kind of cancer cells which demonstrated an excellent selectivity and sensitivity.

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Impedimetric cholera toxin biosensor based on β-galactose derivative functionalized gold surface

정대호 이원용*

연세대학교 화학과

Cholera toxin, an oligomeric complex secreted by Vibrio cholera, which causes dehydration and severe diarrhea due to the binding of B subunits to GM1 ganglioside on the surface of mucous cells in the small intestine. More specifically, cholera toxin is a hexameric protein complex consist of five identical B subunits and an active single A subunit. The five identical B subunits are specifically bind to pentasaccharide ganglioside receptor. It is estimated that 3 to 5 million are infected and approximately 100,000 are killed by cholera per year worldwide. Due to its acuteness, cholera patients require immediate diagnosis and round the clock care. Several analytical methods were developed for CT detection such as fluorescence bioassay and immunoassay. These are based on antibody and GM1 moiety, but they have some limitations such as lack of stability, time-consuming and expensiveness. In the present study, a simple, rapid, label-free and effective cholera toxin biosensor has been developed by using electrochemical impedance spectroscopy (EIS) between modified gold electrode functionalized with synthesized monosaccharide β-galactose and cholera toxin. The present study demonstrates a great analytical performance of β-galactose modified Au electrode in terms of sensitivity and low detection limit as 800 fM which is much lower than the previous study.

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Highly Efficient Electrogenerated Chemiluminescence Phenol Detection based on $Au_{22}SG_{18}$ Nanocluster in Aqueous Solution

김재윤 표경림 이동일 이원용*

연세대학교 화학과

Quantum sized metal nanoparticles have been continuously studied in recent years because of their promising property towards various applications. Among the various metal nanoparticles, nanoparticles composed of gold atoms have attracted wide attention in analytical sciences because they have unique optical and electrochemical properties but are not toxic. Phenolic compounds used in medicals and industrials can be so harmful to human body, especially, to skin, liver and kidney. Therefore, the determination of phenolic compounds is clearly important. There are many analytical methods for determination phenolic compounds such as high performance liquid chromatography, capillary electrophoresis and fluorescence detection. But these methods have some limitations, requiring complex sample pretreatments and long analysis time. In this study, the $Au_{22}SG_{18}$ nanocluster consisted of 22 gold atoms and 18 thiolate ligands has been synthesized and its electrogenerated chemiluminescence (ECL) properties have been characterized in order to detect phenolic compounds using amine compounds as co-reactant. In the present study, ECL of $Au_{22}SG_{18}$ nanocluster was generated in aqueous phase. In addition, highly efficient ECL quenching has been obtained in the presence of phenolic compounds. This experimental results have demonstrated the ECL of $Au_{22}SG_{18}$ nanocluster holding great promise for real analytical sciences.

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Transition Metal Composites of Pt-Ni-Conducting Polymer for Oxidation of Organic Compounds

Abhijit Pandurang Jadhav 심윤보*

부산대학교 화학과

Pt-Ni alloy has been proved as an effective catalyst with high performance in various electrochemical reactions and sensor applications. Pt-Ni composites with conducting polymer can be a potential sensor material for the electrochemical oxidation of organic compounds. However, despite of their outstanding electrocatalytic abilities, large-scale usage of these catalysts containing high amount of Pt remains greatly hindered due to the high cost and low abundance of these metals. Transition metal-based composites have been studied and introduced as potential replacement for Pt. Making a composite of Pt with Ni and conducting polymer can be promising way to reduce the amount of Pt in the catalysts. The microwave-synthesized composites were characterized by XPS, FE-SEM, EDX and electrochemical methods, respectively. The nano-sized composites of Pt-Ni-conducting polymer shows promising application in the oxidation of various organic compounds.

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Multicolored Electrochromic devices based on Prussian blue analogues

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(주)마프로 기술연구소 [1]부경대학교 화학과

Prussian blue(PB, iron hexacyanoferrate(Ⅱ)) is famous for electrochromic(EC) material, known to have : water soluble form, KFeⅢ[FeⅡ(CN)6] and water insoluble form, Fe4Ⅲ[FeⅡ(CN)6)]3.The insoluble Prussian blue(PB) becomes dispersion in aqueous solutions by surface modification with ferrocyanide anions. Prussian blue analogues(M-PBAs, M´k[M″l(CN)6]n, M′ and M″ are transition metal) have similar structure, but it is difficult to make soluble form in the same way.In this study, we synthesized insoluble M-PBA(Cu-PBA, Co-PBA, Ni-PBA and Zn-PBA) nanoparticles by simple precipitation method. The dispersion conditions for thin film coating were optimized by controlling the solvents, additives and binders. The flexible M-PBA films were prepared on PET/ITO substrate by wet coating method and the flexible EC film devices were assembled by the combination of the prepared WO3 and M-PBA electrodes with a polymer-gel electrolyte. WO3/Ni-PBA, WO3/Cu-PBA, WO3/Co-PBA and WO3/Zn-PBA EC devices showed reversible color change between deep blue and various colors. EC devices showed high contrast ratio and durability.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ELEC.P-540**

발표분야: 전기화학

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Separation and detection of Endocrine disruptor compounds using Microfluidic Channel Coupled with an Electrochemical Sensor

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부산대학교 화학과

Phenol and bisphenol analogues were detected and separated using a microfluidic channel device coupled with a novel electrochemical sensor. The electrochemical sensor was fabricated by covalent immobilization of organometallic compounds with lipid onto self-assembled layer of pTTBA AuNPs. Morphology and performance of the sensor was characterized employing FESEM, EDX, XPS, impedance spectroscopy and CV. The analytical condition of the experiment was assessed. The linear range and detection limits of phenol and bisphenol analogues were 0.2nM- 150nM. To evaluate the applicability of the proposed method it was applied to detect Endocrine disruptor compounds in tap water, the result shown the sensor is highly specific and sensitive.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-541**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Electrochemical investigation of High-performance Electrocatalyst coupled with V2O5 Inverse Opal Photoelectrode to improve the Oxygen evolution reaction

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Semiconductor metal oxides are one of the most interesting materials for photoelectrochemical (PEC) applications due to the solar energy is considered as a clean and renewable method for hydrogen production. Vanadium oxide (V2O5, Eg = 2.8 eV) has drawn considerable interest recently because of its surface catalytic properties, optical properties. In this work, we developed 3D inverse opal architecture with Vanadium pentoxide, which has offered the light-harvesting and charge collection properties was performed using the polystyrene opal template with a size of approximately 450 nm. Upon this template, V2O5 inverse opal (IO) film fabricated through spin-coating method.We found that the optimized V2O5 IOs samples yielded the photocurrent density of ~1mA/cm2 vs. NHE in 05M Na2SO4 aqueous solution under 1 sun illumination condition.However, V2O5 Photocatalyst has suffered by the large overpotential that limits the photoelectrochemical performance(PEC). In order to minimize the overpotential, we modified the photocatalyst with an effective electrocatalyst.Subsequently, the role of electrocatalyst and characterization part will be discussed in detail. Keywords: V2O5, Opal template, Photoelectrochemical water splitting, Electrocatalyst.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ELEC.P-542**
발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Spiro-OMeTAD Conductivity Effects on Organometal Halide Perovskite Solar Cells

Kien Vu Trung 오일환[1,*]

금오공과대학교 IT 융합공학과 [1]금오공과대학교 IT 융합공학과, 금오공과대학교 응용화학과

Organometal halide perovskite solar cells (PSCs) have achieved astounding progress in the past few years and a very high recorded power conversion efficiency (PCE) of 22%. Notable achievements of primary device configuration involving perovskite layer, hole-transporting materials (HTMs) and electron-transporting materials (ETMs) are reviewed. However, there does not fully understand the effect of HTMs, here such a lithium bis(trifluoromethylsulfonyl)-imide doped 2,2’,7,7’-tetrakis(N,N-di-p-methoxyphenylamine)-9,9’-spirobifluorene (Spiro-OMeTAD), on PSCs. On the one hand, the loss of performance of PSCs is commonly attributed to degradation of the perovskite itself. On the other hand, it is needed time for LiTFSI-doped Spiro-OMeTAD hole-transporting layer reaching its conductivity stable after fabrication and storage. In this paper, we study the contribution of the conductivity of LiTFSI-doped Spiro-OMeTAD to the overall current-voltage behavior of PSCs. The mechanism of light and air-exposure are also discussed to overcome the critical issues for a suitable progress of PSCs and related opto-electronic deivces.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
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발표분야: 전기화학
발표종류: 포스터, 발표일시: 금 13:00~14:30

Bio-inspired surface modification of porous carbon for high-performance electrochemical capacitor

윤하나[*] 조우경[1,*]

한국에너지기술연구원 분리변환소재연구실 [1]충남대학교 화학과

Porous carbons are recommended as an electrode material for electrochemical capacitors because they have many important properties such as relatively high electrical conductivity, chemical stability, and large specific surface area, which are necessary for enhancing capacitance. Furthemore, to improve the limited capacitance of carbon-based electrochemical capacitor, we coated the surface of carbon electrodes with dopamine hydrochloride. The electrochemical redox reaction of the surface-coated polydopamine gives additional pseudocapacitance contribution, leading to the enhanced capacitance.

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Electrochemical performance modification of organic catholyte materials by molecular tuning

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UNIST 에너지 및 화학공학부 [1]UNIST 에너지공학부 [2]UNIST 나노생명화학공학부

Redox flow batteries (RFBs) are highlighted for large energy storage system, because of cost effective and ease of scalability. Especially, nonaqueous redox flow batteries (NRFBs) are widely studied to overcome problem of low electrochimical window in traditional water based system. Recent NRFB researches are mainly investigating viable redox active material for both electrode, notably, organic redox active materials give great attention to replace inorganic based materials due to environmentally benignancy, structural diversity and chemical tunability, etc. However, existing studies focus on redox site and simple frameworks, research for molecular tuning by functional group is rarely discussed, even though, study for increasing solubility. Molecular tuning by functional group can profoundly affect not only solubility, also electrochemical characteristic. Herein we report 2-phenyl-1,4-naphthoquinone and its derivatives, for organic catholyte of NRFB system. Each derivatives showed different electrochemical performance by position and kind of functional group. Electrochemical performance were characterized with cyclic voltammetry, unique tube type Li metal battery, and theoretical approach by computational method.

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장소: 일산 KINTEX
발표코드: **EDU.P-469**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

과학 중심 해외 봉사활동에 대한 교수들의 이야기

한재영* 차정호[1,*] 홍준의[2]

충북대학교 사범대학 화학교육과 [1]대구대학교 과학교육학부 [2]서원대학교 생물교육과

국립국제교육원에서는 2016 년 교원해외파견사업의 일환으로 해외 단기 교육봉사 프로그램을 운영하는 대학을 처음으로 선정하였다. 이 사업은 한국의 예비 교원들에게 방학 중 해외 교육봉사 기회를 제공하여 글로벌 감각을 갖춘 교원을 양성하고 해외 교육활동을 장려하는 목적을 가진다. ODA 공여국인 한국의 대학생들이 전 세계에 있는 ODA 수원국에 가서 초등학생 및 중등학생에게 교육봉사활동을 4~5 주에 걸쳐 수행하는 것이다. 이 연구는 이 프로그램을 운영하는 4 개 대학의 이야기를 다룬다. 충북대, 대구대, 서원대, 부산대에서는 2016 년 2 학기 겨울방학 기간에 니카라과, 필리핀, 동티모르, 탄자니아로 교육봉사 활동을 나갔으며, 대학생 봉사단을 인솔한 교수들이 이 연구의 참여자가 된다. 네 명의 과학교육 전공 교수들이 해외 봉사활동을 준비하고 수행하고 평가하는 과정에서 경험한 것들을 자기 연구(self-study)의 방법으로 정리한다. 봉사활동 일지, SNS 를 통한 대화, 봉사활동 평가회 등의 자료를 분석하여 해외 봉사활동의 의미와 시사점을 도출한다. 해외 봉사활동을 나가는 이유, 해외 봉사활동에 대한 인식, 교육관이나 교육철학, 교육 봉사활동을 통해 얻는 것과 잃는 것, 해외 교육봉사활동의 좋은 점과 주의할 점, 해외 봉사활동과 과학교육 등의 측면에서 해외 봉사활동에 대해 대한화학회 학술대회 참가자들과 공유하고자 한다.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표코드: **EDU.P-470**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

모델의 이그노런스(Ignorance)를 강조한 교사교육이 과학교사에 미치는 영향

김성기 **백성혜**[1,*]

나주고등학교 [1]*한국교원대학교 화학교육과*

과학에서 사용하는 모델은 그 모델이 설정한 전제조건 안에서만 작동한다. 즉, 과학에서 사용하는 모델은 자연현상 그 자체에 대한 진술이 아니며, 단순화와 근사를 통한 패턴 찾기 등을 통해 만들어진 것으로 실제 자연과는 거리가 있다. 우리가 비유를 이용하여 어떤 과학 개념을 설명할 때, 비유와 실제가 무엇이 다른지 까지를 학생들에게 알려주어야 한다는 것과 같이 과학 모델이 갖는 한계를 명확히 알고 이를 학생에게 전달하기 위해서는 교사가 먼저 그 모델에 대한 이해가 선행되어야 한다. 본 연구는 과학 교사의 모델에 대한 이해를 도와주기 위해 과학 모델이 갖는 이그노런스(ignorance)를 강조한 교사교육을 실시하였다. 과학교사는 자신이 가르치는 과학 모델에 대한 이그노런스를 찾는 활동을 통해 모델에 대한 이해가 높아졌으며, 이를 통해 자신이 이를 학교 현장에서 가르칠 때 유의해야 하는 지도방식에 변화를 갖게 되었다. 이처럼 교사나 예비교사 교육을 실시할 때 과학 모델을 단순히 전달하는 것이 아니라 그 모델의 등장과 모델이 갖는 한계까지 인식할 수 있는 교육이 실시되어야 할 것이다.

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장소: 일산 KINTEX
발표코드: **EDU.P-471**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

대학수학능력시험 화학Ⅰ 선택 및 문항 인식 조사를 통한 화학Ⅰ 응시자 감소 원인 분석

김현경 김재수[1] 박종석[1,*]

강북고등학교 [1]경북대학교

2009 개정 교육과정이 적용된 이후 대학수학능력시험 과학탐구영역에서 화학Ⅰ 과목 응시자가 점차 감소하는 추세이다. 여기에는 여러 가지 원인이 있겠지만 이 연구에서는 대학수학능력시험에서 화학Ⅰ 선택에 대한 인식과 문항 수준에서 그 원인을 찾는다. 이를 위해 화학Ⅰ 문항의 적절성을 분석하고, 화학Ⅰ 선택에 대한 교사와 학생의 인식을 조사한다.

분석 문항은 2014 학년도부터 2016 학년도까지의 대학수학능력시험 화학Ⅰ 문항 중 일부이다. 이 문항을 교육과정의 내용요소 및 성취기준, 성취수준에 적절한지 분석하였다. 인식 조사 대상자는 고등학교 3 학년 452 명과 과학교사 68 명이다.

연구 결과, 화학Ⅰ 문항은 교육과정에서 요구하는 내용의 깊이와 성취수준에 비해 다소 어렵고 복잡한 수학적 사고력이 요구되는 것으로 나타났다. 화학Ⅰ 선택은 본인의 진로, 향후 희망 전공 관련성이 주요인이었다. 화학Ⅰ을 처음부터 선택하지 않았거나 중도에 다른 과목으로 변경하게 된 이유로는 화학Ⅰ을 선택하면 타 교과에 비해 상위 등급을 받기에 불리하고 학습에 대한 부담이 크다는 것이 제시되었다. 화학Ⅰ의 선택여부에 관계없이 화학Ⅰ 문항 풀이에는 수학적 사고력과 복잡한 수리능력이 필요하다고 인식하였다. 또한 교사들은 최저학력기준 충족 면에서 화학Ⅰ 선택이 불리하다고 생각하였고 그에 따라 학생들에게 화학Ⅰ 응시를 권유하는 것에 소극적이었다. 그리고 대부분의 교사들은 화학Ⅰ 문항 출제 방향의 개선이 필요하다고 인식하였다.

화학Ⅰ 선택 인식과 문항 분석으로부터 대학수학능력시험 화학Ⅰ 응시자 수가 줄어드는 이유를 알아본 결과, 화학Ⅰ 문항이 교육과정의 수준 보다 높아서 학생들이 어렵게

인식하였고 수능 등급을 맞추지 못한다는 인식으로 인해 선택이 줄어들었다. 따라서 화학 I 문항을 수학적으로 해결하는 것이 아니라 화학 지식을 활용해서 해결할 수 있는 문항이 출제될 필요가 있다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-472**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

산-염기 학습발달과정 연구 및 검사 도구 개발- 산-염기 모델의 관점 중심으로 -

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학생들은 산-염기를 학습할 때 많은 어려움을 느끼는데, 그에 대한 혼란의 원인으로 다양한 산-염기 모델의 설명방식의 충돌이 제기되었다. 모델은 모델마다 상이한 맥락을 가지며, 그에 따라 동일한 용어의 정의도 달라진다. 예를 들어 아레니우스 산-염기 모델에서 산은 수용액 상태에서 수소이온을 내놓는 물질이기 때문에 물은 산이 될 수 없지만, 브뢴스테드-로우리 모델에서 산은 수소이온을 주는 물질이기 때문에 물은 암모니아에 대해 산으로 작용한다. 그러나 학생들은 이러한 상이한 맥락을 구분하지 못하기 때문에 중성이었던 물이 왜 산이 되는지에 대해 혼란을 느낀다. 지금까지 산-염기 학습 및 대안개념에 대한 많은 연구들이 있어왔으나 기존의 연구들은 산-염기 개념을 중심으로 연구되어 왔다. 그러나 이러한 개념은 모델이라는 설명체계를 기반으로 하고, 따라서 학생들이 산-염기 개념을 이해하기 위해서는 모델의 관점에 대한 발달이 함께 이루어져야한다. 따라서 본 연구에서는 새로운 모델을 학습할 때, 한 모델의 관점에서 새로운 모델의 관점으로 변해가는 과정을 중심으로 산-염기 학습발달과정을 연구하고, 이러한 모델의 관점을 중심으로 산-염기 학습발달 단계를 판단할 수 있는 검사 문항을 만들고자 한다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-473**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

시각장애 중·고등학생의 물의 상태변화 개념에 대한 사례 연구

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이 연구에서는 시각장애를 가진 중·고등학생의 물의 상태변화 개념을 조사하였다. 과천과학관에서 진행한 시각장애학생 대상의 과학 탐구 활동에 참여한 중학생 16 명, 고등학생 15 명(14 명은 전맹, 13 명은 저시력)에게 '물 분자'와 '얼음의 분자구조' 모형에 대한 개별적인 탐색과 연구자 및 참여자와의 대화를 통해 과학탐구 활동을 진행하였다. 활동은 참여자에게 분자모형을 탐색하게 하고 해당 개념을 설명하는 단계로 구성하였으며 모형을 통한 이해와 활용 가치에 대하여 반구조화된 면담을 실시하였다. 모든 대화는 녹음되었고 그 자료를 전사한 뒤 분석하였다. 연구 결과, 시각장애학생들은 활동에 사용된 모형이 무엇으로 어떻게 구성되어있는지 정확히 대답하였지만 무엇을 나타낸 모형인지 설명하기 어려워하였다. 물의 분자와 상태변화에 대해 배운 경험이 있다고 대답하였으나 그 개념에 대해 제대로 설명하지 못하거나 현상적인 경험에 기초한 수준에 불과했다. 활동을 통해 시각장애학생들은 물의 분자와 상태변화에 대해 이해하게 되었고 모형의 필요성과 유용성에 긍정적인 반응을 보였다. 이러한 결과에 기초하여 교육학적 함의를 논의하였다.

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예비 화학교사들의 학습양식과 유기화학 성취도의 상관성

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경상대학교 화학교육과

화학은 관찰 가능한 거시적 세계를 준미시적 수준 해석하며 상징적 표상으로 나타내는 특성이 있다. 화학의 분류는 대상에 따라 유기화학, 무기화학으로 분류하고 방법론적으로는 물리화학, 분석화학으로 분류한다. 학습자의 정보인식, 처리 유형에 따라 과목의 선호도와 성취도의 차이가 나타난다고 보고 되고 있다.유기화학이란 탄소를 포함하는 화합물을 다루며 입체 구조, 전자의 효과에 관심을 가지는 학문이다. 다양한 분야에서 요구 되므로 화학, 생화학, 화공, 재료, 섬유, 식품, 고분자, 신소재, 생물학과, 의대, 치대 등에서도 교육과정에 반영되어 있다. 많은 과에서 개설하고 있는 과목이기에 배우는 학생들의 수는 많지만 적극적으로 참여하는 경우나 흥미를 느끼지 못하거나 어려움을 겪는 경우의 다양한 학생들을 볼 수 있다. 따라서 본 연구에서는 예비 화학교사들을 대상으로 학습양식과 사고양식 분포를 조사하여 학습양식과 사고양식에 따른 유기화학 1 학기의 성취도를 비교 분석하고, 학습양식과 사고양식에 따른 유기화학 1 학기 내용 영역 및 문항유형별 성취도의 차이를 살펴보았다.

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2015 개정 과학 교육과정과 교수·학습 자료에 포함된 8가지 과학 실천 분석: ‘통합과학’ 중심으로

이정원 최애란[1,*]

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2015 개정 교육과정의 과학과 주요 개정 내용 중 하나는 과학적 소양을 함양하고자 고등학교 공통필수 과목인 ‘통합과학’을 신설하고 탐구 역량을 강화하고자 한 것이다. 2015 개정 과학 교육과정에서는 미국 차세대 과학 기준(Next Generation Science Standards)에서 제시한 8 가지 과학 실천과 같은 8 가지 탐구 기능을 제시하여 다양한 탐구 중심의 학습을 강조하고 있다. 이에 본 연구에서는 2015 개정 과학 교육과정 통합과학 과목에 제시된 32 개의 ‘성취기준’, 40 개의 ‘탐구 주제 및 활동(예시)’, 통합과학 교수·학습 자료에 제시된 활동지를 8 가지 과학 실천 및 세부 성취 목표를 기준으로 분석하였다. 분석 결과 교육과정에 제시된 ‘성취기준’에는 조사 계획하고 수행하기, 자료 분석하고 해석하기, 설명 구성하고 문제 방안 고안하기, 증거에 입각하여 논의하기의 실천이 많이 포함되어 있고 ‘탐구 주제 및 활동(예시)’에는 조사 계획하고 수행하기, 자료 분석하고 해석하기, 설명 구성하고 문제 방안 고안하기, 증거에 입각하여 논의하기, 정보를 얻고 평가하고 소통하기의 과학 실천이 많이 포함되었으며 ‘성취기준’에는 부족한 모형 개발하고 사용하기의 과학실천도 제시되었다. 교수·학습 자료에 제시된 활동지에는 교육과정 ‘탐구 주제 및 활동(예시)’와 유사한 경향을 보였으나 모형 개발하고 사용하기의 과학실천이 높은 비율로 제시되었다. 질문하고 문제 규정하기와 수학 및 전산적 사고 이용하기의 과학 실천은 교육과정의 ‘성취기준’과 ‘탐구 주제 및 활동(예시)’, 그리고 교수·학습 자료 활동지 모두에 적게 포함되었다. 이러한 연구의 결과는 현장 과학교사가 2015 개정 과학 교육과정 통합과학 탐구 활동 계획 및 수행 시 고려해야 할 여러 가지 시사점을 제공할 수 있을 것이다.

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장소: 일산 KINTEX
발표코드: **EDU.P-476**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

자유학기제 과학과 수업 방법과 교사의 수업에 대한 인식

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자유학기제는 학생들이 시험부담과 입시경쟁에서 벗어나 자신의 꿈과 끼를 발견할 수 있도록 수업을 운영하는 제도로, 자유학기제 운영 학기에는 교육과정 재구성과 교과수업 방법 개선이 집중적으로 이루어진다. 자유학기제 교과 수업에서는 학생 참여 및 활동 중심의 수업과 수업 방법의 다양화를 강조한다. 또한 자유학기제 수업의 효과적인 진행은 이를 계획하고 실행하는 교사의 인식에 따라 결정된다. 이에 본 연구에서는 2016 년 전국의 중학교에서 자유학기제가 전면 시행된 이후 과학과에서 사용한 수업 방법과 교사들의 과학 수업에 대한 인식을 분석하기 위한 설문 문항을 개발하고자 한다. 설문지 개발과 관련된 선행연구를 분석하여 본 연구의 설문 문항 개발 절차를 수립하였다. 자유학기제 관련 선행연구에서 수업 방법 영역을 고찰하여 하위 항목을 선정하였다. 자유학기제 수업 방법 하위 항목은 교과 내용 재구성, 학생 참여 및 활동 중심 수업, 수업 방법의 다양화, 융합 연계 수업으로 구성하였다. 자유학기제 과학 수업에 대한 교사 인식은 한국교육개발원 '자유학기제 정착 방안 연구' 설문지에서 제시한 교사 인식과 관련된 설문 문항 중 이해, 태도, 고충, 개선사항을 하위 항목으로 구성하였다. 자유학기제 실태와 교사 인식에 관한 선행연구들의 설문지와 면담지 문항으로부터 자유학기제 과학 수업과 수업에 대한 교사 인식에 관련한 설문 문항을 추출하여 하위 항목으로 분류후 재구성하였고, 일부 문항은 본 연구에서 개발하였다. 본 연구에서 개발한 설문지를 자유학기제를 경험한 중등 교사를 대상으로 실시하여 분석하는 후속 연구 계획이 있다.

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발표분야: 화학교육
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자유학기제 과학과 평가 계획 및 시행과 교사의 평가에 대한 인식

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자유학기제는 중학교 과정 중 한 학기동안 학생들이 시험 부담에서 벗어나 꿈과 끼를 찾을 수 있도록 학생 참여형으로 수업을 운영하고, 학생의 성장과 발달을 지원하는 과정 중심의 평가를 실시하는 제도이다. 자유학기제의 취지를 달성하기 위해서는 수업에 상응하는 평가가 연계적으로 이루어져야 한다. 이에 본 연구에서는 2016 년 자유학기제가 전국 중학교에서 전면 시행된 이후 과학과에서의 평가 계획 및 시행과 교사의 과학과 평가에 대한 인식을 조사하기 위한 설문 문항을 개발하고자 한다. 설문지 개발과 관련된 선행 연구 분석을 바탕으로 본 연구의 설문 문항 개발 절차를 수립하였다. 본 연구의 주제인 '자유학기제' 관련 선행 연구를 고찰하여 '자유학기제'의 하위 항목을 선정하였다. 자유학기제는 기본 교과와 자유학기 활동으로 구성되어 있고, 기본 교과의 운영은 학생 중심 교육과정 편성, 참여와 활동 중심의 교수·학습, 과정 중심 평가로 구성되어 있다. 과정 중심 평가에 관한 설문지를 개발하는 본 연구에서는 평가 주체, 평가 내용, 평가 방법, 평가 결과의 4 가지를 하위 항목으로 선정하였다. 자유학기제에 관한 선행 연구의 설문지에서 관련 문항을 추출하여 하위 항목으로 분류 후 재구성하였고, 일부 문항은 본 연구에서 개발하였다. 평가 주체에서는 자유학기제 평가 주체가 교사인지 학생인지 조사하고, 평가 내용에서는 인지적 영역인지 정의적 영역인지 알아보았다. 평가 방법에서는 실제 시행되는 평가 방법을 조사하고, 평가 결과에서는 평가 후 피드백 여부 및 서술식 기재와 관련한 문항으로 구성하였다. 자유학기제 과학과 평가에 대한 교사 인식은 한국교육개발원 '자유학기제 정착 방안 연구'의 구성원의 인식 및 실태 조사 설문지에서 제시한 하위 항목 중 이해, 태도, 고충, 요구 사항의 4 가지 하위 항목으로 구성하였다. 교사 인식 중 이해에서는 자유학기제의 목적과 취지 및 과정 중심 평가에 대해 교사들이 어떻게 이해하고 있는지를 묻고, 태도에서는 평가를 준비하는 자세, 과정 중심 평가에 대한 교사의 만족도,

동료 교사와의 협의에 대한 태도 문항 등으로 구성하였다. 고충에서는 교사가 느끼는 어려움에 대한 문항으로 구성하였고, 요구 사항에서는 교사들이 필요하다고 느끼는 개선 사항으로 구성하였다. 이와 같은 과정을 통해 개발한 설문지를 자유학기제를 경험한 중등 과학 교사를 대상으로 실시하여 그 결과를 분석하는 후속 연구 계획에 있다.

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장소: 일산 KINTEX
발표코드: **EDU.P-478**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

Chemical education using nanoscience : Change of optical properties depending on the particle size

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Nanoscience is one of the most notable topics of modern science. Actually, the field of nanoscience is not included in the regular high school curriculum in Korea, but it could be treated as a very interesting learning topic and it could be used as a good material in schools for gifted students. In this study, we used silver nanoparticles, which are one of the most familiar nanomaterials in the media. It is very interesting to see completely different optical properties of silver particles as they change in size, such as bulk silver, nanoparticles, and nanodots.In this study, we tried to plan a lesson that combines knowledge and technology of various fields such as physics and spectroscopy with chemistry. And it fits well with recent educational trends that emphasize the importance of interdisciplinary research and convergent thinking. This demonstration is a general tutorial for science high school students or gifted talent in chemistry.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-479**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

국가수준 학업성취도 평가 문항에 나타난 과학의 본성 분석

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본 연구에서는 국가수준 학업성취도 평가의 중학교 3 학년 과학과 문항에 나타난 과학의 본성을 분석하고자 하였다. 이를 위해 이영희(2013)가 제시한 4 가지 과학의 본성 개념 틀을 기준으로 2010 년부터 2015 년 까지 시행된 국가수준 학업성취도 평가의 중학교 과학과 240 개 문항을 분석하였고, 각 문항에 대한 학생들의 답지반응을 분석하였다. 과학의 본성 개념 틀의 4 가지 범주는 Ⅰ. 과학 지식의 본성, Ⅱ. 과학 탐구의 본성, Ⅲ. 과학적 사고의 본성, Ⅳ. 과학과 기술 및 사회의 관계적 본성이다.본 연구의 결과는 다음과 같다. 첫째, 과학의 본성 범주 별로 분석한 결과, 범주Ⅰ 28.3%, 범주Ⅱ 63.8%, 범주Ⅲ 4.6%, 범주Ⅳ 3.3%로 과학 탐구의 본성에 관한 문항이 가장 많이 출제되었다. 둘째, 연도별로 살펴보면 2007 년 개정 교육과정이 적용된 2012 년도 문항부터 범주Ⅲ과 범주Ⅳ의 문항이 출제되기 시작하였고, 2009 년 개정 교육과정의 적용으로 '과학의 본성' 영역의 문항이 추가된 2015 년에 범주Ⅳ 문항이 증가하였다. 셋째, 문항 유형 별로 보면 선다형과 서답형 모두 범주Ⅰ과 범주Ⅱ에 해당하는 문항이 많이 출제 되었으나, 범주Ⅲ의 비율은 선다형 보다 서답형 문항에서 더 높게 나타났다. 넷째, 내용 영역별로 분석한 결과 운동과 에너지, 물질, 생명, 지구와 우주 영역에서 모두 범주Ⅰ, 범주Ⅱ 문항이 높은 비율로 출제되었다. 특히 물질 영역의 경우 문항의 73.3%가 범주Ⅱ에 편중되어 있었고 지구와 우주 영역에서 유일하게 과학의 본성 4 가지 범주가 모두 출제되었다. 다섯째, 문항 별 학생들의 답지반응은 범주 IV 문항의 정답률이 가장 높게 나타났고, 범주 III 문항의 정답률이 가장 낮게 나타났다.

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발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

고등학교와 대학교 화학과 교육과정의 연계성에 대한 대학생들의 인식 조사

백은숙 홍훈기*

서울대학교 화학교육과

이 연구는 고등학교와 대학교의 화학과 교육과정의 연계성에 대한 대학생들의 인식을 통해, 현재 시행되고 있는 2009 개정 교육과정의 개선점을 언급하고, 앞으로 시행될 2015 개정 교육과정의 현장 적용에 도움을 주는 데 목적이 있다. 본 연구에서 중점을 둔 부분은 첫째, 고등학교 수업과 대학수학능력시험의 과학탐구영역 선택과목은 각각 무엇이고 선택한 이유는 무엇인지, 둘째, 고등학교와 대학교의 화학과 교육과정의 연계성에 대한 대학생들의 인식은 어떠한지, 셋째, 새롭게 적용될 2015 개정 교육과정에 바라는 점은 무엇인지이다. 연구의 대상은 일반화학 강의를 수강한 화학과 및 화학교육과 대학생 78 명이다. 설문조사에 참여한 대학생들 중 적극적으로 연구에 참여하겠다고 동의한 9 명은 반구조화 심층면담을 하였다. 설문조사와 심층면담 내용을 중심으로 분석한 연구 결과는 다음과 같다. 첫째, 대학생들은 고등학교 수업과 대학수학능력시험에서 과학탐구영역의 과목을 결정할 때, 학교의 상황과 입시에 영향을 받는다. 둘째, 고등학교 '화학'과 대학교 '일반화학'의 내용은 상당 부분 연계되어 있다. 고등학교 '화학Ⅰ'과 '화학Ⅱ'는 단계적인 과목이므로, '화학Ⅰ·Ⅱ'를 모두 이수하는 것이 '일반화학'을 수월하게 학습하는 데 필수적이다. 셋째, 새로운 교육과정이 적용될 때, 시험 위주의 '문제 풀이'보다 화학에 대한 '개념 이해'가 강화되는 것이 중요하다. 이러한 결과를 바탕으로 2015 개정 교육과정이 교육현장에 효과적으로 적용되기 위한 구체적인 교육 방안을 제언한다.

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장소: 일산 KINTEX
발표코드: **EDU.P-481**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

고등학생의 자유탐구 활동 과정에서 사용된 도구의 특징과 어포던스

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이 연구에서는 고등학생의 자유탐구 활동 과정에서 나타나는 도구 사용의 질적인 특징과 어포던스를 탐색하였다. 연구 대상은 과학 동아리 활동에 참여한 고등학교 1, 2 학년 학생 23 명으로, 학생들은 6 개 조로 나누어 7 차시(14 시간)동안 자유탐구를 계획하고 수행하였다. 학생들의 탐구 활동을 녹음, 녹화 및 관찰하였고, 반구조화된 심층 면담을 실시하였다. 준비물 요청서와 조별 활동지도 수집하였다. 연구 결과, 학생들이 탐구 활동에 필요한 도구를 선정하지 못하거나 선정한 도구에 대한 지식이 부족한 경우에는 도구 발생이 이루어지지 못하였다. 학생이 선정된 도구의 어포던스에 익숙하지 않은 경우에는 시행착오를 거치며 도구 발생이 일어날 때까지 탐구 활동이 제한되었다. 도구 발생은 도구의 특성과 제한을 인식하는 단순한 도구 사용인 도구의 수용과 이를 인식하지 않는 체화된 도구 사용인 도구의 전유로 나타났다. 도구의 전유는 도구 사용에 익숙해지기 위한 도구의 수용을 거친 후 이루어졌지만, 도구의 어포던스가 일상생활에서 이미 체득된 도구의 경우 도구의 전유가 곧바로 이루어졌다. 도구의 전유를 통해 도구의 어포던스가 확장되기도 하였지만, 도구의 전유가 도구의 일반적인 어포던스 내에서 이루어지기도 하였다. 학교 과학 탐구에서 도구에 대한 인식의 재고를 위한 시사점을 논의하였다.

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장소: 일산 KINTEX
발표코드: **EDU.P-482**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

과학관 활용 수업을 위한 프로그램이 중등 예비과학교사의 수업 계획 및 실행에 미치는 영향

최숙영 송나윤 노태희*

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이 연구에서는 과학관 활용 수업을 위한 프로그램을 개발하고 이를 예비교사에게 적용하여 그 결과를 분석하였다. 서울 소재의 사범대학에서 화학교재 연구 및 지도법을 수강 중인 예비교사 중 3 명이 연구에 참여하였다. 과학관 활용 수업을 위한 프로그램은 워크숍, 수업 계획 및 시연 그리고 평가회로 구성하였다. 워크숍은 과학관 학습의 특징과 맥락적 학습 모형에 대한 소개 및 활동지 분석으로 진행되었다. 워크숍 후 연구 참여자 3 인에게 방문 전, 중, 후 활동에 대한 활동지를 제작하도록 하였다. 그리고 제작된 활동지를 예비 분석하여 이를 토대로 반구조화된 면담을 실시하였다. 교수 실행은 수강생을 세 집단으로 나누어 연구 참여자 3 인이 각 집단을 대상으로 과천과학관에서 진행하였다. 교수 실행 후에는 집단별로 평가회를 진행하였다. 평가회에서는 수강생이 활동지 제작 기준에 근거하여 평가한 내용을 토대로 연구 참여자와 자유롭게 논의하도록 하였다. 그리고 수업 관찰 및 평가회 내용을 바탕으로 최종 면담을 실시하였다. 자료 분석은 과학관 학습 수행 전략 틀의 요소를 범주로 하여 예비교사들이 제작한 활동지, 수업 촬영 영상, 면담 전사본 등의 모든 자료를 일차적으로 분류하였다. 그 후, 범주별 자료에 대한 재검토 및 논의를 반복하면서 범주를 정교화 하였다.

연구 결과, 과학관 학습 수행 전략 틀 중 대부분의 요소에서 긍정적인 결과가 나타났다. 예비교사는 과학관에 대한 지리적, 심리적 측면을 고려하였고, 소집단 활동을 통해 공동의 산출물을 만들어 내도록 하였다. 또한 학습자의 흥미를 고려하여 전시물을 선정하였고, 학습자에게 선택권을 제시하여 자발적으로 참여할 수 있도록 하였다. 그리고 활동지 문항을 구성할 때 의미 있는 상호작용을 촉진하기 위한 고려가 나타났다. 반면 일부 요소에

대해서는 부정적인 결과를 보였다. 즉, 방문 전, 중, 후 활동 사이의 연계 측면에 대한 고려는 부족하였고, 단순히 개인적인 체험을 발표하는 것에 그쳐 학습자에게 의미 있는 경험을 제공했다고 보기는 어려웠다. 이러한 결과를 바탕으로 중등 예비과학교사 교육과정에서 과학관 활용 수업 전문성 향상을 위한 활용 방안에 대해 논의하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-483**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

협력적 비유 생성 활동에서 나타나는 비유의 변화 과정과 소집단 토론 및 전체 학급 토론의 특징

김민환 권혁순[1] 노태희[*]

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이 연구에서는 협력적 비유 생성 활동에서 나타나는 비유의 변화 과정과 소집단 토론 및 전체 학급 토론의 특징을 분석하였다. 서울특별시에 소재한 고등학교 2 학년 학생들을 대상으로 협력적 비유 생성 활동을 적용한 수업을 진행하였다. 수업은 개별적으로 목표 개념에 대한 비유를 생성하는 개인 비유 생성 단계, 소집단 토론을 통해 비유를 생성하는 소집단 비유 생성 단계, 전체 학급 토론 이후에 소집단 비유를 수정하는 소집단 비유 수정 단계로 구성하였다. 수업을 모두 마친 이후 반구조화된 면담을 실시하였다. 비유의 변화 과정을 분석하기 위하여 개인 비유와 소집단 비유, 수정된 소집단 비유를 비교하였다. 비유 생성 활동을 위한 소집단 토론과 전체 학급 토론의 특징은 분석적 귀납법을 사용하여 분석하였다.

연구 결과, 비유의 변화 과정은 공유 속성이 추가되는 경우, 비공유 속성을 인식하는 경우, 대응 오류가 수정되는 경우 등 세 가지 유형이 나타났다. 각 유형에 따른 구체적인 사례를 제시하였으며 이를 바탕으로 각 유형에 해당하는 비유물의 특징을 논의하였다. 소집단 토론에서 학생들은 여러 개인 비유 중 하나를 선택하는 방식으로 소집단 비유를 생성하였고, 비유를 선택하는 기준은 비유의 설명력, 독창성, 친숙도 등이 있었다. 또한, 학생들은 비유 생성 활동을 주관적이 창의적인 활동이라고 인식하여 비유 생성 활동에서 정서적 부담과 갈등의 요소가 적었다. 전체 학급 토론의 경쟁적인 분위기는 학생들이 비유의 비공유 속성에 주목하게 하였다. 소집단 비유 수정 단계에서 학생들은 비공유 속성을 비유가 갖는 제한점으로 추가하거나 비공유 속성을 갖지 않도록 비유를 변형하는 방식으로 비유를 수정하였고, 새로운 비유를 생성하는 경우는 거의 없었다.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-484**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

Guided Inquiry and Flipped learning model of Chemistry Class for KSA 1st grade students

최은영* 오진호

한국과학영재학교 화학생물학부

We applied the guided inquiry and flipped teaching model to chemistry first grades students with problem focused on worksheet at KSA (Korea Science Academy) of KAIST(Korea Advanced Institute of Science and Technology). Required class circumstances are such that students should study the basic concepts and summarize lecture contents before the class as homework. During the class, students discuss about 6~7 problems provided by the instructor for 20 minutes. This process induces cooperation through group discussion without any competition within the students. It also provide instructor a way to find students thinking ability. After discussion time, within the team of two students, every team has to present the results of their inquiry problem and during such presentation other teams can actively participate and raise some inquires and discuss all together in class of 14~16 students. In this way, peer teaching gives an opportunity to every student to develop his or her presentation skills and inquiry abilities. In addition, this learning model increases student efficiency and confidence in science learning.

일시: 2017년 4월 19~21일(수~금) 3일간
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발표분야: 화학교육
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발성사고법을 활용한 학생들의 비유 생성 과정 조사

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이 연구에서는 발성사고법을 활용하여 학생들의 비유 생성 과정을 심층적으로 조사하였다. 서울특별시에 소재한 고등학교에 재학 중인 2 학년 학생 12 명이 연구에 참여하였다. 학생들은 발성사고법을 활용하여 이온 결합에 대한 비유를 생성하였으며, 이후 반구조화된 면담을 실시하였다. 지속적 비교 방법을 사용하여 비유 생성의 단계를 구분하고 이에 따른 과정 요소를 추출하였다.

연구 결과, 학생들은 비유 생성 과정에서 부호화, 소재 탐색, 대응, 정교화의 네 단계를 거쳤다. 부호화 단계에서는 목표 개념의 하위 속성 중 주요 속성을 선택하는 주요 속성 선정과 선택한 속성을 일상적 용어로 변환하는 주요 유사점 추출의 요소가 나타났다. 소재 탐색 단계에서는 비유의 소재를 선택하는 소재 선택의 요소가 있었고, 소재 평가의 요소를 통해 순환적 과정을 거쳐 최종적인 비유의 소재를 선택하였다. 대응 단계에서는 비유물에 각각 유사점과 차이점을 추가하는 공유 속성 대응과 비공유 속성 대응의 요소가 나타났으며, 유사점을 추가하기 위해 비유에서 표현하고 있는 상황을 수정하거나 새로운 비유의 상황을 가정하는 비유 상황 구체화 요소가 나타나는 경우가 있었다. 정교화 단계에서는 수정이나 철회 등의 요소를 통해 생성한 비유의 정교화가 이루어졌다. 이 연구의 결과를 바탕으로 과학 학습에서 효과적인 비유 생성을 위한 지도 방안을 제안하였다.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-486**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

중등 예비 화학 교사의 지필평가 문항 제작 과정의 특징 분석

노태희 김혜리[1] 한재영[2] 강훈식[3,*]

서울대학교 화학교육과 [1]서울대학교 사범대학 화학교육과 [2]충북대학교 사범대학 화학교육과 [3]서울교육대학교 과학영재교육대학원

이 연구에서는 중등 예비 화학 교사가 지필평가 문항을 제작하는 과정의 특징을 발성 사고법을 이용하여 분석하였다. 이를 위하여 8 명의 예비 화학 교사가 발성 사고법을 통하여 기체 법칙에 대한 6 개의 지필평가 문항을 제작하는 발성 사고 과정과 개별 심층 면담 전사본을 분석하였다. 분석 결과, 예비교사들은 지필평가 문항 제작 과정에서 문항 제작 계획 단계에서의 체계성 부족, 수업과 평가의 상호관련성에 대한 인식 및 고려 부족, 문항 유형 결정 기준의 다양성, 행동 영역과 난이도 판별 곤란, 교사용 지도서 활용의 제한성과 교사용 지도서에 대한 오해, 검토 관점과 내용의 제한성 및 검토시기에 따른 검토 내용의 차이 등의 6 가지 특징을 보였다. 이상의 결과는 예비교사들이 지필평가 문항을 제작하는 과정에서 주로 고려하는 측면과 부족한 측면에 대한 정보를 제공하므로, 예비교사의 지필평가 문항 제작 능력을 향상시키는 방안을 모색하는 데 의미 있는 시사점을 제공할 수 있다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **EDU.P-487**
발표분야: 화학교육
발표종류: 포스터, 발표일시: 목 11:00~12:30

과학관련 사회쟁점 수업에서 스마트 기기의 활용에 따른 특징

<u>남혜인</u> 강훈식[1] 노태희[*]

서울대학교 화학교육과 [1]서울교육대학교 과학영재교육대학원

이 연구에서는 고등학생의 과학관련 사회쟁점(SSI) 수업에서 스마트 기기를 활용함으로써 나타나는 특징을 분석하였다. 경기도에 소재한 고등학교 1 학년 학생들을 대상으로 집단지성원리를 적용한 과학관련 사회윤리적 쟁점수업 모형에 스마트 기기를 적용한 SSI 수업을 진행하였다. 스마트 기기를 활용한 SSI 수업을 자료 탐색 및 공유 과정, 소집단 토론 및 전체 학급 토론 과정, 온라인 토론 과정으로 분류하여 과정별 특징을 분석하였다. 연구 결과, 자료 탐색 및 공유 과정에서 학생들은 자신이 선호하는 형태의 자료를 검색하였고, 자료의 검색과 공유가 동시에 이루어졌다. 또한, 이 과정을 통해 수집한 근거의 다양성과 타당성 및 출처의 명확성이 향상되었다. 소집단 토론 및 전체 학급 토론 과정에서는 정확한 근거에 기반한 주장과 이에 대한 반박이 활발하게 이루어졌으며, 이는 토론에 대한 학생들의 흥미를 높여 학생들의 적극적인 토론 참여로 이어졌다. 온라인 토론 과정에서는 전체 학급 토론에서 수업시간의 한계로 인해 마무리 짓지 못한 내용을 정리할 수 있었고, 전체 학급 토론에서 소극적이었던 학생들의 토론 참여가 높아지는 것으로 나타났다. 이러한 연구 결과를 바탕으로 스마트 기기를 활용한 SSI 수업을 효과적으로 진행하기 위한 방안에 대해 논의하였다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-488**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fate of mustard gas after application to the soil surface

정현숙

국방과학연구소 화생방부

After application of mustard gas (HD) to the soil surface, its possible fate follows evaporation, absorption, and degradation. Using a laboratory-sized wind tunnel, thermal desorber in combination with gas chromatograph-mass spectroscopy (GC-MS), and ^{13}C nuclear magnetic resonance, systematic analysis of the fate of HD was performed. The results show that a drop of neat HD deposited on the soil surface evaporated slowly while being absorbed immediately into the matrix. The initial evaporation or drying rates of the HD drop were power-dependent on its initial drop volume with the smaller drops evaporating relatively quicker. HD absorbed into the soil remained for a month, degrading eventually to nontoxic thiodiglycol via hydrolysis through the formation of sulfonium ions.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-489**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Fenton-like reaction of metal ferrite with chelating agents: Batch and feasibility test

강유경 장윤석*

POSTECH 환경공학부

It has been noticed that some chelating agents can enhance heterogeneous Fenton reactions, as well as homogeneous Fenton reactions. However, the mechanism of the enhanced heterogeneous Fenton reactions remains unclear, due to the ambiguous coexistence of homogeneous and heterogeneous reactions. In the present work, ethylene diamine tetraacetic acid (EDTA) was introduced to study the role of the chelating agent in the oxidation of 4-chlorophenol (4CP) in metal ferrite system. Ferrite has similar structure with magnetite (Fe3O4), which Fe2+ sites were substituted to other metal cations. The presence of some metals in the ferrite structure strongly increased the rate of H2O2 decomposition and the oxidation of the organic molecules. 5 kinds of ferrites were synthesized by co-precipitation method with manganese, cobalt, nickel, copper and zinc. The addition of EDTA in solution accelerated 4CP removal due to the induced homogeneous Fenton reaction by enhanced dissolution of metal cation, and reaction rate was like that (Cu=Ni>Mn>Zn>Co). Meanwhile, the adsorbed EDTA on the catalyst could also enhance 4CP removal. Effects of EDTA surface loadings, chelating agents (EDDS, NTA, oxalic acid and citric acid), initial H2O2 concentrations, initial 4CP concentrations, and initial pH on the reaction kinetics in EDTA modified ferrite/H2O2 system were investigated. Results showed that the surface complexed EDTA (Me2+/Fe3+-EDTA) inhibited H2O2 decomposition by competition for surface active sites. The enhanced 4CP removal by Me2+/Fe3+-EDTA was probably due to the efficient use of reactive oxygen species (ROS). Additionally, field applicability was tested in soil slurry condition using subsurface soil mixed with 4CP spiked solution.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-490**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Recyclable superparamagnetic adsorbent based on mesoporous carbon for sequestration of radioactive Cesium

강유경 장윤석*

POSTECH 환경공학부

Novel and recyclable superparamagnetic adsorbent Fe3O4-O-CMK-3 was synthesized by in situ growth of nanometer sized magnetite particles (m-NPs) on the surface of mesoporous carbon at low temperature (70 °C) using ecologically-benign materials. Structural characterization by transmission electron microscopy (TEM) confirmed the formation of 20 nm thick oxidized mesoporous carbon layers around the magnetic NPs. Thermogravimetric analysis (TGA) results revealed dense carboxylic and phenolic groups on the surface of Fe3O4-O-CMK-3. Because of these abundant polar groups the Fe3O4-O-CMK-3 had stronger adsorption affinity towards Cs than did magnetic mesoporous carbons O-Fe-CMK-3 synthesized by impregnation, and Fe-O-CMK-3 synthesized by co-casting, even in the presence of high concentrations of competing cations (K+, Na+, Li+, Ca2+ and Sr2+). The Fe3O4-O-CMK-3 adsorbent reached a steady state quickly (< 5 min) with maximum adsorption capacity of 205 mg g-1 which is sufficiently higher than other magnetic adsorbents (usually lower than 110 mg g-1) reported in the literature. The synthesized nanostructure adsorbent could be retrieved in a few seconds using an external magnet and reused at least six times for contaminant removal.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-491**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

16-year trend and Exposure Assessment of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans (PCDD/Fs) in outdoor air and human serum in Seoul, Korea

강유경 장윤석*

POSTECH 환경공학부

Polychlorinated dibenzo-p-dioxin/furans (PCDD/Fs) were measured in air and human serum samples collected, respectively, from residences and residents living within a 1 km radius of municipal solid waste incinerators (MSWIs) during a 16-year period from 2001 to 2016 in Seoul, Korea. The mean toxic equivalent (TEQ) concentrations of PCDD/Fs were 0.08 pg TEQ/m3 and 9.90 pg TEQ/g lipid, respectively. Air and serum samples exhibited similar profiles of PCDD/F congeners, and 2,3,4,7,8-PeCDF and 1,2,3,7,8-PeCDD were determined as major congeners. Air sampling was carried out in summer and winter, and the concentrations were 0.03 and 0.12 pg TEQ/m3, respectively. The levels of particle phase were detected about 5 times higher than those of gas phase, and it was also confirmed that the smaller particle size of the particles had the higher concentrations. The dioxin intake rate through respiration was 0.0066 pg TEQ/kg-day, which was lower than the reference value of 0.2 pg TEQ/kg day. The dioxin levels in air during a 16-year period showed a trend of about 95% reduction from 2001 when the dioxin emission regulation were strengthened. About 37% of participants' serum dioxin levels were within the range of 8-10 pg TEQ/g lipid, and the serum dioxin levels for 16 years did not show any significant change. Dioxin levels showed strong positive associations with age, but no correlation with sex or BMI. In addition, diabetic patients had higher dioxin levels than normal people, but there was no statistically significant correlation. This study examined that the effects of dioxin emission sources on human exposure and the longest changes of dioxin in both air and serum in Korea.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-492**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Matrix-specific diastereomeric profile and spatial distribution of hexabromocyclododecane (HBCD) in a multimedia environment

강유경 장윤석*

POSTECH 환경공학부

Hexabromocyclododecane (HBCD) contamination and its diastereomeric profile were investigated in a multi-media environment along a river at the local scale in air, soil, sludge, sediment, and fish samples. The spatial distribution of HBCD in each matrix showed a different result. The highest concentrations of HBCD in air and soil were detected near a general industrial complex; in the sediment and sludge samples, they were detected in the down-stream region (i.e., urban area). Each matrix showed the specific distribution patterns of HBCD diastereomers, suggesting continuous inputs of contaminants, different physicochemical properties, or isomerizations. The particle phases in air, sludge, and fish matrices were dominated by α-HBCD, owing to HBCD's various isomerization processes and different degradation rate in the environment, and metabolic capabilities of the fish; in contrast, the sediment and soil matrices were dominated by γ-HBCD because of the major composition of the technical mixtures and the strong adsorption onto solid particles. Based on these results, the prevalent and matrix-specific distribution of HBCD diastereomers suggested that more careful consideration should be given to the characteristics of the matrices and their effects on the potential influence of HBCD at the diastereomeric level.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-493**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Distribution of various contaminants (PCDD/Fs, DL-PCBs, HBCDs, TBBPA) in singular cow

강유경 장윤석*

POSTECH 환경공학부

Various contaminants have persisted in environmental matrices and affected to ecosystem through the food chain from their sources to human. Especially, the concerned contaminants, emitted by human activity and industrial use, have been studied for their fate and estimated dietary intakes such as polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs), dioxin-like polychlorinated biphenyls (DL-PCBs) and hexabromocyclododecanes (HBCDs), tetrabromobisphenol A (TBBPA). In this study, we investigated various parts of beef and their internal organs from singular cow, and discussed how these contaminants spread to those parts. In the case of meat, muscle parts are more generally monitored as the main edible part rather than internal organs. But various parts including rarely consumed internal organ parts in other countries were also monitored in this study. In the general view of food sampling, meat packing processes are legally managed and prohibited a direct taking-out from the slaughterhouse. Thus, the permission from Korea government should be required for sampling in advance; as a result, we secured a strong point from selection of sample unlike general monitoring studies.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-494**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Human exposure to HBCD via indoor dust

강유경 장윤석*

POSTECH 환경공학부

Human exposure to brominated flame retardants (BFRs) such as hexabromocyclododecane (HBCD) mainly occurs through diet and dust ingestion. In this study, the HBCD concentrations in 124 vacuum dust samples of six indoor environments (homes, offices, kindergartens, cars, schools, and public indoor environments) and 32 surface dust samples were investigated. The median HBCD concentrations ranged from 106.30 ng g-1 in home dust to 496.13 ng g-1 in office dust. The estimated daily intakes (EDI) of HBCD (dust+diet) for toddlers were 6.18 ng kg-1 bw d-1. In general, the ΣHBCD estimated body burden of Korean adults showed good agreement with the reported HBCD median concentrations in their sera. Since the developmental health effect of exposure to HBCD was categorized as “high hazard” by the US Environmental Protection Agency, the estimated high body burden of ΣHBCD in Korean toddlers (9.76 ng g-1 lw) warns us of possible adverse effects on the development of essential systems in their bodies.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-495**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparing removal efficiencies of 1,4-dioxane and Arsenic(III) by nZVI-common oxidant systems

강유경 장윤석*

POSTECH 환경공학부

Nanoscale zerovalent iron (nZVI) activated three common peroxides (persulfate (PS), peroxymonosulfate (PMS) and hydrogen peroxide (HP)) were evaluated for 1,4-dioxane and As(III) removal. The peroxide oxidants are capable of producing radicals when they are coupled with initiators like UV, heat and transition metals. In this study, nZVI was used as an alternative to release Fe(II) and adsorbent for arsenic species. The order of removal efficiencies of 1,4-dioxane and As(III) was PS > HP > PMS with nZVI. Also, the nZVI/PS system showed high efficiency in simultaneous removal of both contaminants. As oxidant concentration increases, the removal efficiency also increased while high nZVI dosage only enhanced As removal. The increasing pH had negative effect to nZVI/oxidant systems due to the lower Fe(II) dissolution from nZVI. In pH 3, Fe(II) dissolution was promoted with three oxidants, especially PS dissolved large amount of Fe ions in presence of As(III) in pH 3 - 7. The promoted corrosion could accelerate removal of As by co-precipitation with Fe ions. The main produced radical was hydroxyl radical (OH·, E0=2.70V),while sulfate radical (SO4•-,E0=2.60V)contributedpartiallyin1,4-dioxaneremoval.The main removal mechanism of As(III) was not an oxidation with radicals, rather by adsorption and co-precipitation. The knowledge gained from this study aids in selecting proper oxidant used with nZVI to purify water/wastewater contaminated by organic/inorganic contaminants.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-496**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Comparative toxicity of surface-modified zerovalent iron nanoparticles on aquatic and terrestrial organisms

강유경 장윤석*

POSTECH 환경공학부

Nanoscale zerovalent iron (nZVI)-based materials are increasingly being applied in environmental remediation, therby lead to their exposure to aquatic and terrestrial biota. However, little is known regarding the fate and ecological effects of nZVI, particularly of surface-modified nZVI. In this study, we compared the toxicities of different forms of nZVIs, such as bare nZVI, carboxymethyl cellulose (CMC)-stabilized nZVI, tetrapolyphosphate (TPP)-coated nZVI, and bismuth (Bi)-doped nZVI, on a range of aquatic and terrestrial organisms, including bacteria (Escherichia coli and Bacillus subtilis), plant (Arabidopsis thaliana), water flea (Daphnia magna), and earthworm (Eisenia fetida). Bi- and CMC-nZVI induced adverse biological responses across all test systems, except E. fetida, that varied from cell death in E. coli, B. subtilis, to inhibition of the physiological state in D. magna and A. thaliana. The particle characterization under exposure conditions indicated that surface modification of nZVI played a significant role by changing their physicochemical properties and therefore, their toxicity. The underlying mechanism by which nZVI induces toxicity may be a combination of oxidative stress and cell membrane destabilization and/or the toxic effect of bismuth itself. Overall, our findings provide important implications in the development of environment-friendly nZVI materials and direct further research regarding interspecies exploration

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-497**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Structural engineering of metal free carbon nitride polymers with benzene doping for enhanced photocatalytic activity under visible light

김혜진 최원용*

POSTECH 환경공학부

Graphitic carbon nitride (g-C3N4) have attracted much attention as a polymeric visible-light photocatalyst. However, the limited visible light absorption and fast electron-hole recombination have restricted its photocataytic efficiency. To overcome this drawbacks, grafting aromatic groups onto the surface of g-C3N4 is investigated to extend the delocalization of the π electrons and change the intrincic semiconductor properties. Here, we advanced this strategy by synthesizing the carbon nitride substituted nitrogen of tertiary amine to benzene connected by three heptazine rings. The intramolecular benzene doping by simple method induced the structural distortion that is calculated theoretically and when increasing the benzene doping concentration, amorphization is also progressed. This structural changes of carbon nitride bring about remarkably enhanced charge separation of photogenerated electron-hole pairs and red-shift of the optical absorption. As a result, the modified carbon nitride showed increased photocatalytic efficiency on the degradation performance of organic pollutant and hydrogen peroxide generation under the visible light (λ > 420 nm). This study offers simple strategies to induce chemical and structural change of the carbon nitride only consisted of earth-abundant elements for enhanced photocatalytic activity.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-498**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Optimization of hydrogen release from ammonia borane by using plasmonic photocatalyst: Gold deposited TiO2

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POSTECH 화학공학과 [1]POSTECH 환경공학부

Hydrogen has been considered as a promising alternative energy source. However, storage of Hydrogen has been a big problem to fuel cell system. As a solution, hydrogen storage solid materials have received a lot of researcher's attention. Among the reported hydrogen storage solid materials, especially, ammonia borane (AB) drew much attention because it has many advantages (e.g. low molecular mass (30.87 g/mol), high hydrogen capacity (19.6 wt%) and stability in solid state) compared with other materials. In addition, in the presence of an appropriate catalyst, AB can in principle produce 3 equivalent moles of hydrogen gas by a hydrolytic decomposition reaction. In this study, optimization condition of hydrogen generation from the decomposition of AB is studied by applying Au-TiO2 plasmonic photocatalyst under visible light irradiation. TiO2 can only absorb ultraviolet light, owing to its large bandgap (~3.2 eV). However, when the gold nanoparticles are deposited on TiO2 surface, it can absorb visible light due to surface plasmon resonance(SPR) of gold nanoparticles. The decomposition of AB is studied under visible light irradiation due to the absorption efficiency of the prepared catalyst, Au-TiO2. 1 wt% of Au-TiO2 supported on three different types of TiO2 viz. anatase (ST-01), rutile and P25, are employed to compare their photocatalytic performances. In addition, different amount of gold photo-deposited and 1 wt% of gold impregnated ST-01 are also tested for comparison. Among these photocatalysts, 1 wt% of gold photo-deposited ST-01 produces 85 μmol of hydrogen and it shows the best photocatalytic activity, because Au1ST-01 has the largest surface area and fewer recombination centers. This research will be a fundamental base for optimization of photocatalytic activity by using various metal-metal oxide heterojunction photocatalysts.

일시: 2017년 4월 19~21일(수~금) 3일간

장소: 일산 KINTEX

발표코드: **ENVR.P-499**

발표분야: 환경에너지

발표종류: 포스터, 발표일시: 목 11:00~12:30

New Type of Metal Chelating Coordination Sites in Polymeric Carbon Nitride: Enhanced and Stable Photocatalytic Activities Under Visible Light

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We report a novel and simple approach to introduce a new kind of metal coordination site in polymeric carbon nitride (CN) by a simple keto-enol cyclization route of acetylacetone and urea, which results in the successful incorporation of metal chelating pyrimidine derivative into the molecular framework of CN. Further introduction of various metals into this coordination site induced significant enhancements in visible light photocatalytic activities as compared to those of pure carbon nitride and the conventional “nitrogen pot” metal-coordinated carbon nitride. It should be noted that the optimized metal loading on carbon nitride was as low as ~0.16 wt %, which is markedly lower as compared to any metal-incorporated CN catalysts reported in the literature. The photocatalyst activities were assessed for both 4-chlorophenol (4-CP) degradation and H_2 production under visible light (λ>420). The Al-functionalized CN displayed the significantly higher activity of 4-CP removal and mineralization as compared to pure CN and other kinds of metal ions incorporation (e.g., Li^+, Mg^{2+}, Ta^{5+}) exhibited similar results. On the other hand, the photocatalytic activity for H_2 production sensitively depended on the kind of metal ion incorporated and the Li-incorporated samples showed the highest activity.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-500**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Long-lasting antibacterial and antibiofouling effects of water-based paint containing silver nanoparticle-decorated silica hybrid particles

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The prevention of bacterial contamination is of great interest because bacterial infections can cause a serious threat to public health. The use of antimicrobial coating materials may inhibit the growth of bacteria. Silver nanoparticles (AgNPs) are well known for their high antibacterial effect, but aggregate severely in aqueous media. We have made silver nanoparticle-decorated silica hybrid particles (AgNPs@SiO2) that were well-dispersed and retained their unique structure and morphology in water-based paint without any aggregations. (0.2 wt%) The release of silver ions (Ag+) from paint film was slow and steady for more than 2 years when tested in distilled water. The paint film containing AgNPs@SiO2 showed excellent antibacterial effect by killing both gram positive bacteria (S. aureus) and gram negative bacteria (E. coli). In addition, antibiofouling property was observed in the natural surface water which was collected from Jeongleung stream. The hybrid particle AgNPs@SiO2 is expected to be a promising antibacterial additive.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-501**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

염소 및 브롬 산화제의 자외선 광분해 수처리에서 pH에 따른 수산화 라디칼 산화 효율과 할로겐 부산물 생성

이유리 이우림 이윤호*

GIST 지구환경공학부

정수처리장, 수영장, 양식장 등 다양한 수처리 시설에서 잔여 산화제 농도를 줄이고 오염물질의 제거효율을 강화시키기 위해 할로겐 산화제(염소산화제/브롬산화제)와 UV 공정을 결합시키는 경우가 늘어나고 있다. 할로겐 산화제는 UV 에 의해 광분해 되면서 라디칼이 발생한다. (HOX + UV → ·OH + ·X, X=Cl, Br) 발생된 라디칼은 높은 오염물질과의 반응성으로 오염물을 빠르게 분해시키기도 하지만, 산화제와 다시 반응하여 chlorate, chlorite, bromate 와 같은 무기 소독부산물을 발생시킨다. 그 중에서도 bromate 는 발암물질로서 기준치가 10 ppb 로 굉장히 낮다. 그러므로 본 연구에서는 140 μM 의 산화제를 UV 조사하였을 때, 1) 염소산화제와 브롬산화제의 광분해 속도 2) 라디칼에 의한 오염물의 제거 효율 및 발생특성 3) 무기 소독부산물 발생에 대해 연구하고자 하였다. UV 에 의한 할로겐 산화제의 광분해는 1 차 반응으로 진행되고, 할로겐 산화제의 분해는 HOCl>OCl->HOBr>OBr- 순으로 빠르게 일어난다. OBr-의 몰흡광계수가 다른 할로겐 산화제 종들에 비해 현저히 작으므로 광분해 속도도 낮다. 산화제의 광분해로 인해 발생된 라디칼에 의한 Benzoic acid 의 분해속도 상수는 cm2 mJ-1 의 단위로 HOCl(8.0×10-3)>HOBr(2.1×10-3)>OCl-(5.9×10-4)>OBr-(8.4×10-5)순이며, 할로겐 산화제 종간 최대 10 배 정도의 차이를 보인다. 과량의 tert-butanol 을 주입하였을 때 라디칼과의 반응을 통해 발생한 formaldehyde 의 발생 수율은 종간 최대 2 배의 차이를 보였다. 이는 오염물 제거효휼의 차이가 할로겐 산화제의 광분해로부터 발생하는 일차 라디칼 발생의 차이 때문이 아니라, 라디칼과 할로겐 산화제의 반응 속도 차이 때문이라는 점을 시사한다. 또한 할로겐 산화제와 라디칼과의 반응으로 발생하는 무기 소독부산물의 발생 수율은 염소산화제의 경우 pH 와 무관하게 ~7%

정도였으나, 브롬산화제의 경우에는 pH 에 따라 큰 차이를 보이며 HOBr 이 ~9%, OBr-가 ~3%로 측정되었다. 과량의 tert-butanol 을 주입하였을 때에는 발생한 라디칼과 tert-butanol 의 반응성이 더 우세하여서 무기 소독부산물의 발생이 1% 미만으로 억제되었다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-502**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Deactivation of antibiotic resistance gene during (photo)chemical oxidative water treatment with chlorine, UV and UV/$H_2 O_2$

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GIST 지구환경공학부

Recently, antibiotic resistant bacteria (ARB) and antibiotic resistance gene (ARG) have been identified as emerging contaminants of concern in aquatic environments as they can spread antibiotic resistance through horizontal gene transfer among bacterial populations (Dodd, 2012). Oxidation processes have been widely used for water disinfection and can be an important barrier for limiting the spread of ARB. However, concern exists for the potential transfer of intact remnants of ARG to bacterial cells by gene transformation process (which does not require live donor cells). Currently, limited information exists for the deactivation efficiency of ARGs during oxidative water treatment (McKinney and Pruden, 2012). This study examined the potential of chlorine, UV, and UV/$H_2 O_2$ to deactivate pUC4K plasmid encoding ampicillin and kanamycin resistant genes as a model ARG .The plasmid in extracellular form as well as the plasmid present in a host E. coli were examined in parallel to see the effect of the bacterial cell components on the ARG deactivation efficiency. An extended amplicon-length quantitative polymerase chain reaction (qPCR) assay was used to determine ARG damage events. Deactivation experiments were performed in phosphate buffered and wastewater effluent matrices.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-503**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced transformation of atenolol during water treatment with chlorine and UV: roles of N-Cl photolysis

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Atenolol, a b-blocker and trace organic contaminant found in drinking water sources, is poorly eliminated in water chlorination despite of the high reactivity of its secondary amine moiety toward chlorine forming N-Cl atenolol. It has been shown that N-Cl atenolol is readily back-transformed to the parent structure in post de-chlorination step with sulfite. The transformation of atenolol can be significantly enhanced when chlorination is followed by UV (Cl2 + UV) or combined with UV irradiation (UV/Cl2) due to the photolysis of N-Cl atenolol. To better understand the fate of atenolol during water treatment with chlorine and UV, this study investigated the kinetics and products of the UV photolysis of N-Cl atenolol. The fluence-based first-order transformation rate constant of N-Cl atenolol was 2.2´10-3 cm2/mJ (kUV,atenolol= 3´10-5 cm2/mJ), indicating that the N-Cl moiety can be significantly photo-transformed at typical UV doses for UV-based advanced oxidation process (e.g., >100 mJ/cm2). Several transformation products were identified by LC-QTOF-MS analysis from the photolysis of N-Cl atenolol, such as products with m/z of 225, 239 and 265. The formation of these products could be explained by 1) N-Cl photolysis and formation of the N-centered radical, 2) radical shift from the N to the neighboring carbons, 3) peroxyl radical formation via oxygen addition, and 4) imine formation and hydrolysis. Implications of the findings from this study will be discussed with regard to the transformation of amine-containing compounds during water treatment with chlorine and UV.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-504**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

N-nitrosodimethylamine (NDMA) formation during chlorination and ozonation of N,N-dimethylhydrazine compounds: Reaction kinetics, mechanisms and implications for NDMA formation control

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Compounds with N,N-dimethylhydrazine moieties ((CH3)2N-N) form N-nitrisodimethylamine (NDMA), which is a suspected human carcinogen, during ozonation, but the relevent reaction chemistry is hitherto poorly understood. This study investigated the reaction kinetics and mechanisms of NDMA formation during chlorination and ozonation of daminozide (DMZ) as structural model N,N-dimethylhydrazine compounds for a more generalized prediction of NDMA formation in various water qualities and ozonation treatment conditions. Pre-chlorination as mitigation strategies against NDMA was also tested. The reaction of ozone with DMZ was fast (kO3 5 105 M-1s-1 at pH 7). Molar NDMA yields (i.e., Δ[NDMA]/Δ[precursor] 100) were 100% for DMZ in the presence of tert-butanol as hydroxyl radical (·OH) scavenger. The molar NDMA yield decreased significantly in the absence of tert-butanol, indicating ·OH formation and its subsequent reaction with the parent precursors forming negligible NDMA. The reaction of with DMZ was relatively slow (k·OH 3.4 × 109 M-1 s-1 at pH 7). The reaction mechanism in the reaction of DMZ with ozone was proposed, forming NDMA as a final product. The reaction of DMZ with chlorine was moderately fast (kHOCl 60 M-1s-1 at pH 7) and gives no NDMA as product. Chlorinated byproducts of DMZ did not form NDMA in ozonation, Overall, significant NDMA formation was found to be unavoidable during ozonation of water containing N,N-dimethylhydrazine compounds due to their rapid reaction with ozone forming NDMA with high yield, while pre-chlorination can be an effective measure to minimize the NDMA formation during ozonation of water containing N,N-dimethylhydrazine compounds.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-505**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

페레이트(Fe(VI))를 이용한 산화수처리에서 요오드 이온의 반응 경로 및 요오드계 소독부산물 생성 제어 가능성

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정수처리 공정에서 수중에 iodide 존재 시 다양한 산화제(오존, 염소, 클로라민)와의 반응을 통해 빠르게 HOI 를 생성하게 되는데, 오존을 제외한 다른 산화제들은 HOI 와의 반응성이 없거나, 매우 느리다고 알려져 있다. 이때 HOI 는 수중의 용존유기물(DOM)과의 반응을 통해 아이오도포름(CHI3)과 같은 요오드 계열의 소독 부산물(I-DBPs)을 발생 시킨다. 이러한 소독 부산물 생성을 최소화하기 위해 본 연구에서는 페레이트라는 산화제의 적용가능성을 평가하였다. 페레이트와 iodide 및 HOI 와의 반응속도 상수를 측정하였으며, 반응경로를 규명하였다. 페레이트와 iodide 간의 반응은 중성 pH 에서 높은 속도 상수 (kapp > 10,000 M-1s-1)를 보이며, pH5 이하에서는 속도상수가 더 증가하는 경향을 보였고, 반면, pH8 이상에서는 반응속도상수가 급격히 감소하는 경향을 보였다. 이러한 경향은 pH 에 따른 Fe(VI)의 종분화로 설명할 수 있다. 중성 pH 에서 과량인 HFeO4-와 낮은 pH 에서의 H2FeO4 는 iodide 와 높은 반응성을 보이지만, FeO_4^{2-}는 iodide 와 반응성이 낮기 때문에 높은 pH 에서는 pH 가 증가함에 따라 반응속도가 감소하는 경향을 보인다. 하지만, pH9 에서 kapp 가 500 M-1s-1 으로 여전히 높은 반응속도상수를 보였다. 다른 산화제들은 iodide 와의 반응이 빠르더라도, HOI 와는 상대적으로 느리게 반응하였지만, Fe(VI)의 경우 HOI 와 더 높은 반응성을 보였다. pH8.5 에서 kapp 가 10,000M-1s-1 으로 매우 빠른 반응을 보였으며, pH8.5 이하에서는 수기로 반응속도상수 측정이 불가할 정도로 빠르게 반응하였다. HOI 는 페레이트에의해 iodate 로 산화되는 한편, iodide 가 검출되기도 하였다. 이러한 반응은 페레이트에 의해 가속화된 HOI 의 불균화 반응(IO2- + HOI => IO3- + I- + H+)과 Fe(VI)와 HOI 반응 시 생성된 과산화수소에 의한 HOI 의 환원반응으로 설명 가능하다. 결론적으로,

Fe(VI)는 iodide 및 HOI 와 높은 반응성을 가지며, 최종 부산물로 무해한 iodate 를 생성하기에, 처리될 물에 iodide 존재시 Fe(VI)를 전산화제로 활용한다면, I-DBPs 생성 억제에 크게 기여 할 수 있다.

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-506**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

제올라이트와 활성탄, 알루미나를 포함한 질소, 인 동시 제거용 다공성 복합소재 개발

김중일 최원석*

철원플라즈마산업기술연구원 신소재&전략기획본부

최근 도시화, 산업화로 인한 수계에 질소 및 인의 유입으로 수중 생태계가 파괴되는 현상이 증가하고 있다. 이러한 문제점을 해결하기 위해 본 연구는 수중의 질소, 인 동시제거를 위한 제올라이트와 활성탄, 알루미나를 바인더와 배합하여 제환공정을 거쳐 구형 비드 형태의 다공성 복합소재 개발하는 것이다. 우선 각 소재별 질소, 인 제거율을 확인하기 위하여 NH_4-N 20 mg/L, NO_3-N 20 mg/L, PO_4-P 2 mg/L 의 초기농도, 반응시간 60 분을 기준으로 제올라이트는 선택적으로 NH_4-N 을 83.4%, 알루미나는 PO_4-P 을 95.9%, 활성탄은 NO_3-N 86.3%,PO_4-P 을 67.3%의 제거율을 나타내었다. 이를 근거로 제올라이트와 알루미나, 활성탄을 바인더와 배합하여 구형 비드형태를 갖는 다공성 복합소재를 제조하여 동일한 농도조건과 시간으로 제거율을 측정하였을 때 NH_4-N 85.8%, NO_3-N 63.8%, PO_4-P 72.3%의 제거율을 보였으며, 흡착 종료 후에도 구형의 형태를 유지하여 회수가 가능한 다공성 복합소재를 개발하였다. 이러한 특성을 통해 본 연구를 통해 개발된 다공성 복합소재는 하수처리장 내 질소, 인 고도처리용 소재로 활용이 가능할 것으로 기대된다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-507**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of MgO Particles and Porosities on Carbon adsorbent for CO_2 Capture

허영정 박수진*

인하대학교 화학과

In this work, magnesium oxide (MgO)-modified carbon adsorbents were fabricated using a nitrogen-enriched carbon precursor by microwave-assisted irradiation for CO_2 capture. On optimising the conditions, the prepared sample attained a high CO_2 uptake of 1.22 mmol/g (5.3 wt.%) under flue gas conditions (15% $CO_2$2 in N_2). It was found that MgO pariticles affected the CO_2 capture behavior by improving the fundamental characteristics of the carbon surfaces.

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일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-508**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Effect of microporosity and surface chemistry on PAN/PVDF-based carbon adsorbents for CO_2 capture

허영정 박수진*

인하대학교 화학과

In this work, PAN/PVDF nanofibers were used as a porous carbon precursor for CO_2 capture. Electrospinning method was used for getting carbon nanofibers and physical activation was adopted for the activation of electrospun carbon nanofibers. The effect of steam activation in electrospun carbon fiber was investigated in relation to textural properties and CO_2 capture and CO_2 /N_2 separation.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-509**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Enhanced bromate reduction by humic substances in ice

민대위 최원용[1,*]

POSTECH 환경공학과 [1]POSTECH 환경공학부

Bromate (BrO_3^-) is an important disinfection by-product (DBPs) formed during ozonation which is nowadays recognized as a carcinogenic and persistent pollutant. Reducing bromate into bromide is an essential process for detoxifying this toxic pollutant, however, not many studies have been done yet. In this work, we demonstrate a new transformation pathway that bromate could be efficiently reduced by freezing the bromate solution in the presence of organic reductants like humic substances. The results show that the amount of eliminated bromate for 1day reaction is 30~40% in dark condition and 80~90% in irradiation condition ($\lambda > 300$ nm) in frozen solution, while less than 5% bromate is reduced in aqueous solution. This significant enhancement in ice is due to the freeze concentration effect. XPS measurement shows the oxidation of humic substance during bromate reduction in frozen solution. Photoluminescence revealed the electron transfer from organic compounds to bromate is much enhanced in frozen condition. These results suggest that freezing process in icy environment would provide unique chemical circumstance for reduction of persistent pollutant in nature.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-510**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

허니컴 구조체 촉매의 메탄 이산화탄소 개질 반응에 대한 상업적 활용 가능성에 대한 연구

김승연

고등기술연구원 에너지환경연구팀

메탄 이산화탄소 개질 반응에 사용되는 촉매에 관한 연구는 주로 촉매와 지지체 사이의 상관관계에 따른 촉매 활성 증가 연구가 주를 이루었다. 하지만, 촉매의 상업적 활용을 위해, 촉매의 성형에 관한 추가적 실험이 필요하다. 이에 본 연구는 추가적 성형이 필요 없는 허니컴 구조체를 지지체로 사용하여, 메탄 이산화탄소 개질 반응용 촉매를 제조했다. 건식코팅방식 중 원자층증착법의 장점인 기공 구조 코팅 가능성과 기상화학증착법의 장점인 대면적 코팅이 가능성을 모아 하이브리드 방식의 Temperature Regulated-Chemical Vapor Deposition (TR-CVD) 방법을 이용하여 촉매를 제조했다. 이렇게 제조된 허니컴 구조 촉매를 메탄 이산화탄소 개질 반응에 대한 활성을 평가함으로서, 촉매의 상업적 활용 가능성에 대하여 확인했다.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

일시: 2017년 4월 19~21일(수~금) 3일간
장소: 일산 KINTEX
발표코드: **ENVR.P-511**
발표분야: 환경에너지
발표종류: 포스터, 발표일시: 목 11:00~12:30

Diffusive gradient in thin films technique for assessing labile mercury fraction in soils

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In this study, we used the diffusive gradients in thin films (DGT) to understand how soil properties (i.e., organic matter content) affect partitioning behaviors of Hg between soil particles and pore water. The accumulated mass of Hg in DGT gel and soil pore water was monitored for 10 days with variable Hg concentrations from 1 to 50 ppm and variable soil peat moss contents from 5% to 20%. Using these experimental data, we were able to estimate T_c (response time) and K_d (distribution coefficient between soil and pore water) as a kinetic and equilibrium parameter, respectively, of Hg using the DGT induced fluxes in sediments and soils (DIFS) model, and k_1 (DGT uptake rate constant) and k_2 (DGT elimination rate constant) using the one compartment model (OCM). When Hg concentration in soil increased from 1 to 50 ppm, T_c values were 1s for all cases and K_d values decreased from 4060 to 407 cm^3g^{-1}. Using the same data, the OCM predicted that k_1 decreased from 3.27×10^{-6} to 5.58×10^{-7} kg soil cm^{-2} d^{-1} and k_2 increased from 1.45×10^{-1} to 4.41×10^{-1} d^{-1} along with increases in Hg concentration. When the soil peat moss content increased from 5 to 20%, T_c increased from 1 to 22 s, and K_d decreased from 63.7 to 6.7 cm^3g^{-1}. Using the same experimental data, the OCM predicted that k_1 decreased from 1.62×10^{-5} to 6.63×10^{-6} kg soil $cm^{-2}d^{-1}$, and k_2 increased from 1.03 to 2.77 d^{-1} while peat moss content increased. These results indicate that the mobilization rate of Hg from soil to DGT tends to decrease with increasing organic matter content, which could be a result of the strong binding of Hg to the soil organic matter. The combined approaches of DGT, DIFS and OCM allow us to obtain better understanding on the partitioning of Hg involved in soil retention and mobilization, suggesting that these methods are suitable tools to predict metal bioavailability in soils.

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The photodemethylation of methylmercury in seawater: the influence of dissolved organic matter

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The methylmercury (MeHg) photodemethylation (PD) with dissolved organic matter (DOM) can occur via two potential pathways in seawater: PD by photochemically produced reactive intermediates (PPRIs; 1O2, ^{3}DOM*, e-aq, ·OH) and direct PD of MeHg-DOM complexes. We investigated the mechanisms of DOM mediation by measuring photodemethylation rate constants (kpd) in artificial seawater under UV-A (365 nm), in the absence/presence of Suwannee River Humic Acid/Fulvic Acid (SRHA, SRFA), Pony Lake Fulvic Acid (PLFA). A predominance of MeHg-SRHA species increased the kpd by 2-5 times that of MeHgCl. The kpd for SRHA was 0.010 h-1, and it decreased to 0.0057 h-1 (·OH quencher) and 0.026 h-1 (1O2 quencher). In similar, the kpd was 0.016 h-1 for PLFA, and it decreased to 0.0125 h-1 (·OH quencher) and 0.0085 h-1 (1O2 quencher). These results imply that microbial FA has higher photosensitization effects than terrestrial HA, and 1O2 is more important than ·OH. Additional experiments with model compounds showed that the PD rate was higher by an order of magnitude in the presence of aromatic thiols (thiosalicylic acid, TA, 0.37 h-1) than aromatic carboxyls (salicylic acid, SA, 0.010 h-1) or nonaromatic thiols (glutathione, GT, 0.019 h-1). It was interesting to find that the kpd were lower in ·OH quencher (0.0066 h-1 for GT, 0.0055 h-1 for SA) than with the 1O2 quencher (0.012 h-1 for GT, 0.0074 h-1 for SA) for nonaromatic thiols and aromatic carboxyls. The kpd for aromatic thiols were similar for both quenchers (0.45 h-1 for 1O2 quencher, 0.40 h-1 for ·OH quencher) and these values were comparable to those determined without quenchers, implying that the role of PPRIs is not significant. Overall, direct PD of MeHg-DOM complexes via intramolecular charge transfer is suggested as a major mechanism for aromatic thiol, while PD by PPRIs is suggested for natural HA/FA. Further studies are necessary to identify effects of 3DOM* by using 3DOM* quencher.

대한화학회 제119회 총회 및 학술발표회 (The 119th General Meeting of the Korean Chemical Society)

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Hybrid mesoporous Cu_2ZnSnS_4 (CZTS)?TiO_2 photocatalyst for efficient photocatalyticconversion of CO_2 into CH_4 under solar irradiation

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A major concern facing global society is the ongoing excessive release of CO_2 into the atmosphere where it acts as a heat-trapping greenhouse gas. One approach to helping control atmospheric CO_2 concentrations is to use solar energy to convert CO_2 into useful products, namely hydrocarbons, by use of specifically designed photocatalytic materials. While numerous photocatalysts have been investigated for use in CO_2 reduction, the field remains in it's infancy with, overall, relatively poor photoconversion efficiencies and product selectivity. This study reports 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. A maximum methane production rate of 118.75 ppm · g^{-1} · h^{-1} is observed, which represents a methane evolution rate approximately 12 times greater than that of pure TiO_2. The key factors contributing to the enhanced photocatalytic performance seen in the mesoporous CZTS–TiO_2 samples include improved light absorption, high surface area, and effective charge separation.

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Catalytic removal of p-nitrophenol by water treated coal fly ash

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A huge amount of fly ash (FA, around 9 million tons per year) has been produced from coal-fired thermal power plants in Korea. To recycle the FA and apply to environmental remediation technologies, we investigated the feasibility of FA as an use of environmental catalysts in this study. A significant reduction of p-nitrophenol (p-NP) to p-aminophenol (p-AP) was observed by ultra-pure Water treated FA (WFA) in the presence of NaBH4, while raw fly ash (RFA) showed a relatively low catalytic activity. We also observed totally different behaviors between FA and WFA, resulting in inhibition effect on the p-NP reduction by increase of FA contents as compared to that of WFA (enhancement effect). To elucidate the reaction mechanism, we synthesized artificial FAs by mixing major components of FA and performed the p-NP reduction, showing that Al2O3, SiO2, CaO and MgO revealed no significant catalytic activity, but Fe2O3 did. In addition, a various parametric tests has been performed to investigate the effect of environmental factors on the catalytic reduction of p-NP in the presence of NaBH4, Finally, five times recycling test showed a good reusability of WFA, indicating the potential use of WFA for the treatment of wastewater containing reductively degradable pollutants.